Formulae for Solutions to (Possibly Degenerate) Diffusion Equations Exhibiting Semi-Classical and Small Time Asymptotics

by

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Table of Contents

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Summary

We derive formulae valid up to the appearance of caustics for a classical solution $f^\mu(t,q)$ of the following Cauchy problem for the diffusion equation on a manifold , which explicitly give the semi-classical ($\mu \to 0$) asymptotics to any desired order and a probabilistic representation of the remainder :

$$\frac{\partial}{\partial t} f^\mu(t,q) = K^\mu f^\mu(t,q)$$
$$f^\mu(0,q) = T_0(q)\exp\left(\frac{-S_0(q)}{\mu^2}\right)$$

where $K^\mu = \mu^2 L + Y + W + \frac{V}{\mu^2}$, with L a smooth scalar second order semi-elliptic differential operator , Y a smooth vector field and V, W, S_0 and T_0 are smooth real valued functions .

Also we derive formulae under a no-caustics assumption for p(t,x,y) , the fundamental solution (heat kernel) , with respect to the natural Riemannian measure induced by a smooth scalar second order elliptic operator L , of the following diffusion (heat) equation on a manifold, that explicitly give the small time ($t \to 0$) asymptotics to any desired order and a probabilistic representation of the remainder :

$$\frac{\partial}{\partial t} f(t,x) = Lf(t,x) .$$

§0 Introduction

(0.0) In **Elworthy and Truman** [2] a probabilistic representation of the minimal solution to the following Cauchy problem for the diffusion equation on a Riemannian manifold :

$$\frac{\partial f^{\mu}(t,q)}{\partial t} = \frac{1}{2}\mu^2 \Delta f^{\mu}_t(q) + \frac{1}{\mu^2}V(q)f^{\mu}_t(q)$$

$$f^{\mu}(0,q) = T_0(q)\exp\left(-\frac{S_0(q)}{\mu^2} \right)$$

where Δ denotes the Laplace-Beltrami operator and V, S_0 and T_0 are real valued functions , was obtained using the Feynman-Kac-Girsanov Formula . This representation was valid up to the time any caustics might appear and the first 'W.K.B.' term in the semi-classical ($\mu \to 0$) asymptotics was easily obtained from it . A further probabilistic representation was obtained , using the same technique , from which the second term in the semi-classical expansion could be obtained but only in the case $T_0 = 1$. The second term was computed in **Watling** [1] following the suggested technique of using **Elworthy and Truman** [1] by localising about the classical path and using the Stochastic Taylor's Formula of **Azencott** [2] but computing in a canonical manner : fortunately this rather complicated approach soon became superseded .

In **Truman** [1] and **Elworthy and Truman** [1] the 'W.K.B.' term before any appearance of caustics in the semi-classical ($\hbar \to 0$)

asymptotics of the solution of the Schrödinger Equation analogous to the above diffusion equation, that is replace μ^2 by $i\hbar$, was obtained using a semigroup of unitary operators. It was observed in **Watling** [2] that this method could be extended rather easily to give the semi-classical asymptotics to any required order : this has since been generalised to obtain the semi-classical asymptotics to any required order for the Schrödinger Equation in a magnetic field on a Riemannian manifold in **Elworthy, Truman and Watling** [1].

In **Watling** [3] a method inspired by the method used for ~~the~~ Schrödinger Equation was devised which generalised the results of **Elworthy and Truman** [1] to a more general class of differential operators on a manifold than $\frac{1}{2}\mu^2\Delta + \frac{V}{\mu^2}$, namely $\mu^2 L + Y + W + \frac{V}{\mu^2}$, where L is a scalar second order semi-elliptic differential operator, Y is a vector field and W is another real valued function. The motivations behind this class of operators are firstly by analogy with the Schrödinger Equation in a magnetic field giving us the Y and W, secondly from the problems of random perturbations of Dynamical Systems and small time asymptotics of hypoelliptic operators giving us the L. Formulae were obtained which explicitly give the semi-classical asymptotics to any desired order and a probabilistic representation of the remainder : these are given in §5. More recently **Doss** [3] has obtained an asymptotic expansion when $M=R^d$, L

may be expressed in Hörmander form as $\frac{1}{2}\sum X_i^2$ and $W=0$, but his methods are rather different , not so explicit or as clearly semi-classical : that is the asymptotics expressed purely in terms of the associated classical mechanics .

In **Elworthy and Truman** [2] and **Elworthy** [1] a probabilistic representation of the heat kernel $p(t,x,y)$ of $\frac{1}{2}\Delta + V$ on a Riemannian manifold with a pole at y , where Δ denotes the Laplace-Beltrami operator and V is a real valued function was obtained by a limiting argument from the formula mentioned above for a carefully chosen Cauchy problem . The leading small time ($t \to 0$) asymptotic could trivially be obtained from it . The formula itself involved a 'Bridge' process which was called the Brownian Riemannian Bridge as it was dependent on the Riemannian geometry and is not the same as the usual bridge obtained by conditioning using the kernel itself . The problem of small time asymptotics even for the more general class of hypoelliptic operators has of course been extensively studied by numerous authors : for example **Molchanov** [1] , **Kifer** [1] , **Pinsky** [1] , **Azencott et al** [1] , **Bismut** [1] , **Taniguchi** [1] , **Ikeda and Watanabe** [1] , **Léandre** [1]-[2] and **Kusuoka and Stroock** [1]-[3] . However the emphasis here (motivated by consideration of the Schrödinger equation) is on obtaining exact formulae for $p(t,x,y)$ which do not lose any information : for example involve all the geodesics not just any minimal one , which is all that is relevant in the small time asymptotic expansion approximations to p(t,x,y) .

In **Watling** [4] the methods devised in **Watling** [3] were applied to derive formulae for the heat kernel p(t,x,y) of a smooth scalar second order elliptic operator L on a manifold when the induced Riemannian manifold has a pole at y . These formulae give the small time asymptotics explicitly to any desired order and a probabalistic representation of the remainder which involves a 'bridge' process which was called a Semi-Classical Bridge Process since it depends on the classical mechanics associated with L and generalises the Brownian Riemannian Bridge Process : these formulae are given in §7 . The method used to derive these formulae make the relationship with the usual conditioned process clearer and are more probabalistic than those used in **Elworthy and Truman** [2] who derive the first formula in a special case .

These formulae may be extended to the case that the exponential map is a covering map in a similar manner to **Elworthy** [1] (Chapter IX §12 Remark 12D (i)) and **Arede** [1] : so in particular we can obtain such formulae for Cartan-Hadamard manifolds and connected nilpotent Lie groups . Moreover the terms in the exact expressions will still give the correct terms in the small time asymptotic expansion approximations to $p(t,x,y)$ on more general complete manifolds : where there is a unique minimal geodesic between x and y along which they are not conjugate (in other words x is not on the cut locus of y) , because by Varadhan's Estimate (see **Azencott et al** [1]) the asymptotic behaviour only depends on the behaviour in a neighbourhood of this geodesic .

The technique in **Watling** [4] has been used by **Ndumu** [1] to obtain formulae exhibiting small time asymptotics for heat kernels in geodesic charts and the original Cauchy technique was used again in **Elworthy, Truman and Ndumu** [1] to obtain heat kernel inequalities and the classical limit of the quantum partition function .

(0.1) In §1 we define the principal symbol , A , of a smooth scalar second order differential operator, L , its associated field of quadratic forms , Q , and whence the meaning of semi-ellipticity and ellipticity . We describe the natural Riemannian metric , g , associated with an elliptic L and its associated natural connection ∇ . We show how L is split into canonical zeroth , first and second order parts by the choice of a connection and then discuss how a Hörmander decomposition of L may be obtained . Finally we give the Stratonovich correction term to convert between these two decompositions of L which give Itô and Stratonovich stochastic differential equation representations for the associated diffusion .

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(0.2) In §2 we recall the natural symplectic structure on T^*M, how it is used to define a vector field for a given Hamiltonian and whence Hamilton's Equation . We define $J(s,p)$, which will be seen to be essentially the action of the classical path through p in T^*M over time s , and investigate its derivatives . We then define the K^μ - Hamiltonian associated with our operators K^μ . We describe the idea of a no-caustics condition , the Cauchy and Kernel systems and their associated no caustics conditions . Then we prove the main result of this section namely the Hamilton Jacobi Theorem for these systems under the corresponding assumptions . Finally we prove a proposition which will be used frequently in the following .

(0.3) In §3 we define the Lagrangian associated with a given Hamiltonian : in particular the K^μ - Lagrangian and whence the action of a path . We state the well known relationship between solutions of Hamilton's Equation , solutions of Newton's equation and extremals of the action functional when our K^μ - Hamiltonian is non-degenerate , and remark that this is not generally true when we allow degenerate K^μ - Hamiltonians . We then give a formula for the action of a classical path and whence the interpretation of J in §2 . Assuming we have a Hörmander decomposition of L we then proceed , inspired by the work of **Bismut** [1] , to describe the conditions under which we have a relationship between our Hamiltonian and Lagrangian

Mechanics . We define the deterministic Malliavin covariance matrix and prove that its invertibility is actually a property of the pair (L,Y) not depending on which Hörmander decomposition is being used . We give a Lie Algebra condition that ensures invertibility along all the paths we require . We give another description of the action functional adapted to a Hörmander decomposition . We show how we can obtain the control function to obtain projections of solutions of Hamilton's equation . Then we prove the main result of the section that under appropriate conditions we can obtain any minimum of the action functional as a projection of a solution of Hamilton's Equation . Finally we give another description of the action of a classical path that will prove to be significant later on .

(0.4) In §4 we define a semi-classical semigroup , evaluate its derivatives and so obtain a probabilistic representation . We then investigate its small μ limit and give an alternative expression in the case when L is elliptic .

(0.5) In §5 we derive formulae exhibiting the small μ asymptotics of the solution $f^{\mu}(t,q)$ of the Cauchy Problem assuming a no caustics condition . We remark that given an appropriate large deviations result that the asymptotics remain true though not of course the formulae provided that there is only one point of Γ_t above q for which the action is an absolute minimum and it does not lie on a fold .

However one of the motivations for this investigation is the analogy with the Schrödinger equation for which all the classical paths are relevant not just those that attain an absolute minimum of the action and so the use of large deviation theory is somewhat against the spirit of this analogy and what should be aimed for is a global formula true in more general circumstances for which all classical paths are relevant from which the asymptotics of the Schrödinger equation can be deduced and the diffusion equation can be proved .

(0.6) In §6 we define another semi-classical semigroup , evaluate its derivatives and so obtain a probabilistic representation . Finally we investigate what this implies for $K^{\mu} = \mu^2 L$ where L is elliptic .

(0.7) In §7 we define a function $q(t,x,y)$ under a no-caustics condition motivated by §6 associated with an elliptic L with which we essentially condition the diffusion . So we define a conditioned semigroup for which we evaluate the derivatives and a conditioned process that we can use to represent the semigroup that we prove is radially the same as a Brownian Bridge . We obtain a formula for the kernel of L in terms of an expectation of a functional of the conditioned process . Then we proceed to derive the main result of this section namely formulae exhibiting small time asymptotics with remainders expressed in terms of expectations of functionals of the conditioned process . We finish the section with a couple of examples indicating the use of the formulae we have just derived .

(0.8) In §8 we give a couple of very simple examples that indicate the problems that arise when you want to derive formulae exhibiting small μ asymptotics for kernels of more general operators under a no caustics assumption and make a couple of conjectures whilst indicating a few more . The same remarks concerning large deviations also apply to these conjectures namely the asymptotics remain true if there is a unique minimising classical path that does not start at a fold in the lagrangian submanifold Γ_t .

§1 Some Notes on Scalar Second Order Differential Operators on Manifolds

(1.1) Let L be a smooth scalar second order differential operator on a smooth d-dimensional manifold M . L may be represented locally in a coordinate chart $x=(x^1,\dots,x^d)$ by :

$$(1.1.1)\quad L(x) = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(x)\frac{\partial^2}{\partial x^i \partial x^j} + \sum_{i=1}^{d} b_i(x)\frac{\partial}{\partial x^i} + c(x)\,,$$

where $a_{i,j}$, $1\le i,j\le d$; b_i , $1\le i\le d$ and c are smooth scalar valued functions on the domain of the chart , and the dxd matrices $(a_{i,j}(x))$ are symmetric .

Let us denote by $\Pi:T^*M\to M$, $\pi:TM\to M$ and $\underline{\Pi}^n:\underline{\mathbb{R}}^n\equiv M\times\mathbb{R}^n\to M$ the cotangent , tangent and trivial product bundle respectively .

(1.2) Definition

The Principal Symbol , A , of L is the section of the bundle of symmetric bilinear maps $L(T^*M,T^*M;\underline{\mathbb{R}})$ defined as follows : for $q\in M$, $p_i\in T^*M_q$ take a smooth function $f_i:M\to\mathbb{R}$ with $f_i(q)=0$ and $df_i(q)=p_i$ for $i=1,2$ then $A(q)(p_1,p_2)=L(f_1f_2)(q)$.

It should be noted that A is well-defined : that is , it does not depend on the choice of such f_i . If L were represented locally in a chart as in (1.1.1) then A(x) would be represented in the same chart by the matrix $(a_{i,j}(x))$. We can also view A as a section of the bundle of linear maps $L(T^*M;TM)$, a section of the tensor bundle $TM \otimes TM$, or even as a bundle morphism from T^*M to TM.

(1.3) Remark

Notice that if A is a bundle isomorphism, then we have a natural pseudo-Riemannian structure, $g: M \to L(TM, TM; \mathbb{R})$, defined by: $g(q)(v_1, v_2) = \langle A(q)^{-1}(v_1), v_2 \rangle_q$, for $q \in M$ and $v_1, v_2 \in TM_q$, where $\langle \cdot, \cdot \rangle_q$ denotes the duality between T^*M_q and TM_q. If L were represented locally in a chart as in (1.1.1) then $g(x)$ would be represented in the same chart by the matrix $(g_{ij}(x)) = (a_{ij}(x))^{-1}$.

(1.4) Definition

The field of quadratic forms $\{Q_q: T^*M_q \to R \mid q \in M\}$ associated to L is defined by: $Q_q(p_q) = \frac{1}{2}\langle p_q, A_q(p_q) \rangle_q$, for $q \in M$ and $p_q \in T^*M_q$. If L were represented locally in a chart as in (1.1.1) then Q_x would be represented in the same chart by the matrix $\frac{1}{2}(a_{ij}(x))$. We also view Q as a real valued function on T^*M.

(1.5) Definition

L is said to be semi-elliptic if the associated quadratic forms are all positive semi-definite and elliptic if they are all positive definite.

(1.6) Remark

(1.6.1) If L is elliptic then A is a bundle isomorphism and the natural pseudo-Riemannian structure , g , on M defined in (1.3) is actually Riemannian and we have the corresponding Riemannian norm $\|.\|$ defined by , $\|v\|=\sqrt{g(v,v)}$, for $v\in TM$. Thus $Q(p)=\frac{1}{2}\|v\|^2$, where $v=A(p)$, $p\in T^*M$.

(1.6.2) Also notice that Grad(f)=A(df) , where f is a scalar valued function on M and Grad denotes the Riemannian Gradient .

(1.6.3) Furthermore we have a natural choice of connection : the 'Levi-Civita' connection , that is the unique torsion free connection compatible with the Riemannian structure .

(1.7) Definition

The zeroth part of L , which we will denote by U is the scalar valued function on M defined by : $U = L(\mathbb{1})$, where $\mathbb{1}$ is the constant function with value 1 . If L were represented locally in a chart as in (1.1.1) then U would be represented in the same chart by the function c . We will denote $L - U$ by L_0 to indicate that it annihilates constant functions .

(1.8) Suppose we are given L and a connection ∇ ; we can then define the first and second order parts of L in an intrinsic manner : i.e. depending only on the connection not on any particular local representation of L . Let $A(\nabla)$ denote the second order part , $X_0(\nabla)$

the first order part (which is just a vector field) and ∇ also denote the covariant derivative associated with the connection , then : $A(\nabla)(f)(q)=\frac{1}{2}$ trace $A(q)(\nabla df)(q)$, where ∇df , the covariant derivative of df is viewed as a section of $L(T^*M;TM)$, and $X_o(\nabla)= L_o - A(\nabla)$. If L were represented locally in a chart as in (1.1.1) and $\Gamma^k_{i,j}$ denotes the Christophel symbols of the connection in the same chart then $A(\nabla)$ would be represented by the scalar second order differential operator :

$$(1.8.1)\quad A(\nabla)(x) = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(x)\frac{\partial^2}{\partial x^i \partial x^j} + \sum_{k=1}^{d}\Big(\frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(x)\Gamma^k_{i,j}(x)\Big)\frac{\partial}{\partial x^k} ,$$

and $X_o(\nabla)$ by the vector field :

$$(1.8.2)\quad X_o(\nabla)(x) = \sum_{k=1}^{d}\Big(b_k(x) - \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(x)\Gamma^k_{i,j}(x)\Big)\frac{\partial}{\partial x^k} ,$$

(1.9) Remark

If L is elliptic and ∇ is the Levi-Civita connection of (1.6.3) then observe that : $A(\nabla) = \frac{1}{2}\Delta$, where Δ denotes the Laplace-Beltrami operator associated to the Riemannian structure of (1.3) .

For the rest of this section we assume L is semi-elliptic .

(1.10) By a simple application of Whitney's Embedding Theorem and the well known result on Euclidean Space , see for example **Ikeda and Watanabe** [1] (Proposition 6.2(ii)) , we can obtain at least a locally Lipshitz section X of $L(\mathbb{R}^n;TM)$, where of course $n \leq 2d+1$, so that if X^* denotes the dual section of $L(T^*M;\mathbb{R}^n)$, then for all $q \in M$, $A(q)=X(q)X^*(q)$.

(1.11) Remark

We have the following relation between Q and X^* :

$Q_q(p_q)=\frac{1}{2}|X^*(q)(p_q)|^2$, where $q \in M$, $p_q \in T^*M_q$ and $|\,.\,|$ denotes the Hilbert norm on $\mathbb{R}^n$. We can also view X^* as an $\mathbb{R}^n$ valued function on T^*M .

(1.12) Remark

(1.12.1) If $\mathbb{L}$ is elliptic the isometric embedding theorem of Nash , see Nash [1] , gives us an isometric embedding $f=(f_1, \ldots ,f_n):M \to \mathbb{R}^n$, where of course we now only have $n \leq \frac{1}{2}(3d^3+14d^2+11d)$, from which we can construct an $X:M \to L(\mathbb{R}^n;TM)$ from linear combinations of the vector fields $X_i = \text{grad}(f_i)$; so we can actually choose a smooth surjective X and hence a smooth injective X^* .

(1.12.2) If $\|.\|$ is the Riemannian norm of (1.6.1) observe that $\|v\| = |X^*(p)|$, where $v = A(p)$ and $|\,.\,|$ is the Hilbert norm on $\mathbb{R}^n$.

(1.13) Given an orthonormal basis $\{e_i \mid 1 \leq i \leq n\}$ of $\mathbb{R}^n$ we may define the (at least locally Lipschitz) vector fields X_i on M by $X_i(q)=X(q)(e_i)$. If we could actually take X to be smooth , which we certainly can when $\mathbb{L}$ is elliptic as remarked in (1.12.1) , then we could actually define the scalar second order semi-elliptic differential operator : $L_X^2 = \sum X_i^2$.

Note that as indicated this depends only on X and the Hilbert space structure of R^n not on the particular orthonormal basis chosen .

If L were represented locally in a chart as in (1.1.1) and $X_i(x)$ by $\sum_j X_i^j(x) \frac{\partial}{\partial x^j}$ then L_X^2 would be represented as the scalar second order semi-elliptic differential operator :

$$(1.13.1) \quad L_X^2(x) = \sum_{i,j=1}^{d} a_{i,j}(x) \frac{\partial^2}{\partial x^i \partial x^j} + \sum_{k,j=1}^{d} \Big(\sum_{i=1}^{n} X_i^j(x) \frac{\partial X_i^k(x)}{\partial x^j} \Big) \frac{\partial}{\partial x^k} \, ,$$

Thus by assuming greater regularity for X we can also decompose L as : $L = \frac{1}{2} L_X^2 + X_e(X) + U$, where $X_e(X)$ is a vector field on M that would be represented in the chart above by :

$$(1.13.2) \quad X_e(X)(x) = \sum_{k=1}^{d} \Big(b_k(x) - \frac{1}{2} \sum_{j=1}^{d} \sum_{i=1}^{n} X_i^j(x) \frac{\partial X_i^k(x)}{\partial x^j} \Big) \frac{\partial}{\partial x^k} \, .$$

and U is as in (1.7) . This 'Hörmander' decomposition will however depend on the choice of X ; and even in the elliptic case there is no natural choice of such an X . However this kind of decomposition is invariant under diffeomorphisms of the manifold .

(1.14) Remark

In the elliptic case however we have a natural choice of such an X for the horizontal lift of L to O(M) the total space of the orthonormal frame bundle , see **Elworthy** [1] (Chapter VII example 1A(iii)) , moreover this X is injective .

(1.15) If we are given a connection ∇ and we can choose a smooth X then the relationships between our differential geometric and Hörmander decompositions are :

$$X_o(X) = X_o(\nabla) - \mathrm{Strat}(\nabla,X)$$

$$\tfrac{1}{2}L_X^2 = A(\nabla) + \mathrm{Strat}(\nabla,X)$$

for : $\mathrm{Strat}(\nabla,X) = \frac{1}{2}\mathrm{trace}\,\nabla X(X(.))(.)$, where ∇X the covariant derivative of X is viewed as a section of $L(TM;L(\mathbb{R}^n;TM))$ and the trace uses the Hilbert space structure of $\mathbb{R}^n$. With the notation of (1.8) and (1.13) $\mathrm{Strat}(\nabla,X)$ may be represented in the above chart by the vector field :

$$(1.15.1)\ \mathrm{Strat}(\nabla,X)(x) = \frac{1}{2}\sum_{k,j=1}^{d}\Big(\sum_{i=1}^{n} X_i^j(x)\frac{\partial X_i^k}{\partial x^j}(x) - \sum_{i=1}^{d} a_{i,j}(x)\Gamma^k_{i,j}(x)\Big)\frac{\partial}{\partial x^k} ,$$

This vector field $\mathrm{Strat}(\nabla,X)$, known as the 'Stratonovich' correction term is used to convert between a differential geometric 'Itô' stochastic differential equation representation of the diffusion process associated with L and its differential topological 'Stratonovich' form associated with a Hörmander decomposition of L : see **Elworthy** [1] .

§2 Some Hamiltonian Mechanics

(2.1) Recall that we have a natural symplectic structure on T^*M given by the non-degenerate exact two-form ω , which is the exterior derivative of the Liouville , or canonical , one-form α defined by : $\alpha(Z)=\langle\pi(Z),T\Pi(Z)\rangle$, for $Z\in TT^*M$, where $\pi:TT^*M\to T^*M$ is the tangent bundle to the total space of the cotangent bundle and $T\Pi:TT^*M\to TM$ is the derivative of $\Pi:T^*M\to M$.

If $x=(x_1,\ldots,x_d)$ is a chart of M and $(y,x)=(y_1,\ldots,y_d,x_1,\ldots,x_d)$ is the associated chart of T^*M then α and ω are represented in this chart by the forms :

(2.1.1) $\alpha(y,x) = \sum y_i dx^i$,

(2.1.2) $\omega(y,x) = \sum dy_i \wedge dx^i$.

Notice that (y,x) give local Darboux coordinates for T^*M considered as a symplectic manifold .

(2.2) This Liouville form is characterised by the following two properties :

(2.2.1) It annihilates the vertical subbundle .

(2.2.2) Every one-form , β , on M satisfies $\beta= \beta^*\alpha$, where β^* denotes pullback via β .

(2.3) Given a smooth Hamiltonian $H:T^*M\to\mathbb{R}$, the symplectic structure is used to define the associated Hamiltonian vector field Z_H on T^*M by : $Z_H = \omega(-dH)$,where ω is viewed as a bundle isomorphism from T^*T^*M

to TT^*M . Z_H is represented in our Darboux coordinates by the vector field :

$$Z_H(y,x) = \sum_i \frac{\partial H}{\partial y_i}\frac{\partial}{\partial x^i} - \sum_i \frac{\partial H}{\partial x^i}\frac{\partial}{\partial y_i} .$$

(2.4) The classical path associated with H from $p \in T^*M$ will be the maximal solution $\theta_{(\cdot)}(p):[0,\tau(p))\to M$ of Hamilton's equation :

$$\frac{d}{ds}\theta_s(p) = Z_H(\theta_s(p))$$
$$\theta_0(p) = p$$

where $\tau(p)$ denotes the explosion time of the solution . This equation is locally represented in our Darboux coordinates by the system of equations :

$$\frac{d}{ds}y_i(s) = -\frac{\partial H}{\partial x^i}(y_1(s),\ldots,y_d(s),x^1(s),\ldots,x^d(s)) \text{ , for } 1\le i\le d$$

$$\frac{d}{ds}x^i(s) = \frac{\partial H}{\partial y_i}(y_1(s),\ldots,y_d(s),x^1(s),\ldots,x^d(s)) \text{ , for } 1\le i\le d$$

$$y_i(0) = y_i \text{ , for } 1\le i\le d$$

$$x^i(0) = x^i \text{ , for } 1\le i\le d$$

where $(y_1(s),\ldots,y_d(s),x^1(s),\ldots,x^d(s))$ and $(y_1,\ldots,y_d,x^1,\ldots,x^d)$ represent $\theta_s(p)$ and p respectively .

(2.5) In the notation of above define the following function for $p\in T^*M$ and $s<\tau(p)$:

$$J(s,p)=\int_0^s \alpha(Z_H(\theta_r(p)))-H(\theta_r(p))\,dr\ .$$

We shall see in §3 that this is essentially the classical action of the projection onto M of the classical path through p .

(2.6) Lemma

We have for $p\in T^*M$ and $s<\tau(p)$:

(2.6.1) $\frac{\partial}{\partial s}J(s,p)=\langle(\theta_s^*\alpha)(p),Z_H(p)\rangle-H(p)$

(2.6.2) $dJ_s(p)=(\theta_s^*\alpha)(p)-\alpha(p)$

Proof

Firstly we make the general remark that if θ is the flow of a vector field Z then :

(2.6.3) $Z(\theta_s(p))=T\theta_s(p)(Z(p))$, since :

$\frac{d}{dr}\theta_r\theta_s(p)=\frac{d}{dr}\theta_s\theta_r(p)$, so

$Z(\theta_{r+s}(p))=T\theta_s(\theta_r(p))(Z(\theta_r(p)))$,

and whence result by taking $r=0$.

This means that :

$$J_s(p)=\int_0^s \langle(\theta_r^*\alpha)(p),Z_H(p)\rangle-(\theta_r^*H)(p)\,dr\ .$$

(2.6.1) So clearly : $\frac{\partial}{\partial s}J(s,p)=\langle(\theta_s^*\alpha)(p),Z_H(p)\rangle-H(p)$

as H is constant along a solution of it's Hamilton's Equation .

(2.6.2) Moreover we see that :

$$dJ_s(p) = \int_0^s \theta_r^*(d(\alpha(Z_H))-dH)(p)\,dr \text{ , as } d \text{ and } \theta_r^* \text{ commute ,}$$

$$= \int_0^s \theta_r^*(L(Z_H)(\alpha)(p)\,dr \text{ ,}$$

where $L(Z_H)$ denotes Lie derivative in the direction Z_H : using **Abraham and Marsden** [1] (2.4.13(iv)) and the facts that in their notation $\iota(Z_H)(d\alpha)=\iota(Z_H)(\omega)=-dH$ and $d(\iota(Z_H)\alpha)=d(\alpha(Z_H))$.

$$= \int_0^s \frac{d}{dr}((\theta_r^*\alpha)(p))\,dr \text{ ,}$$

from the definition of Lie derivative .

$$= (\theta_s^*\alpha)(p)-\alpha(p) \text{ .}$$

□

(2.7) Given a vector field Y on M we define the Hamiltonian $H_Y:T^*M\to\mathbb{R}$ by : $H_Y(p_q)=\langle p_q,Y(q)\rangle$, for $q\in M$, $p_q\in T^*M_q$,and whence the vector field $\underline{Y}$ on T^*M which is the 'complete lift' of Y by $\underline{Y} = Z_{H_Y}$. If Y is represented in a chart by $\sum_i Y^i(x)\frac{\partial}{\partial x^i}$ then $\underline{Y}$ is represented in the corresponding Darboux coordinates by the vector field :

$$Y(y,x) = \sum_i Y_i(x) \frac{\partial}{\partial x^i} - \sum_{i,j} y_j \frac{\partial Y^j}{\partial x^i} \frac{\partial}{\partial y_i} .$$

(2.8) The Hamiltonian Classical Mechanics associated with the second order differential operator $K^\mu = \mu^2 L + Y + W + \frac{V}{\mu^2}$ where L is a smooth scalar second order differential operator , Y is a smoooth vector field , and V and W are smooth scalar valued functions on M , is governed by the Hamiltonian $H: T^*M \to \mathbb{R}$ defined by : $H = Q + H_Y + V \circ \pi$, giving the corresponding Hamiltonian vector field : $Z_H = Z_Q + Y + Z_{V\circ\pi}$. If L is semi-elliptic we will refer to such a Hamiltonian as a K^μ - Hamiltonian and if L is elliptic we will refer to the K^μ - Hamiltonian as non-degenerate . If L were represented locally in a chart as in (1.1.1) then Z_Q and $Z_{V\circ\pi}$ would be represented in the corresponding Darboux coordinates by the vector fields :

$$Z_Q(y,x) = \sum_i \Big(\sum_j a_{i,j}(x)\, y_j \Big) \frac{\partial}{\partial x^i} - \frac{1}{2} \sum_i \Big(\sum_{j,k} \frac{\partial a_{j,k}}{\partial x^i}(x)\, y_j\, y_k \Big) \frac{\partial}{\partial y_i} ,$$

$$Z_{V\circ\pi}(y,x) = - \sum_i \frac{\partial V}{\partial x^i} \frac{\partial}{\partial y_i} .$$

Observe that for a K^μ - Hamiltonian we have : $\alpha(Z_H) = 2Q + H_Y$, as $Z_{V\circ\pi}$ is vertical , and so :

$$(2.8.1)\ J(s,p) = \int_0^s Q(\theta_r(x)) - (V\circ\pi)(\theta_r(p))\, dr .$$

(2.9) Suppose we are given a Hamiltonian , H , and a Lagrangian submanifold , Γ_0 , of T^*M : that is an embedded submanifold of dimension d with ω vanishing on it's tangent space . We could ask whether the following condition on this system is satisfied :

The no-caustics condition :

There exists an interval $I \subseteq \mathbb{R}$ with non-empty interior having $0 \in \mathbb{R}$ as its lower end point so that :

(2.9.1) for all $p \in \Gamma_0$ and $t \in I$, $\theta_{-t}(p)$ exists (i.e. the solution of Hamilton's equation for -H starting at p does not explode until after time t) ,

(2.9.2) The Lagrangian submanifolds Γ_t for $t \in I$ given by $\Gamma_t = \theta_{-t}(\Gamma_0)$ have the property that $\pi_t = \pi | \Gamma_t : \Gamma_t \to M$ is a diffeomorphism .

(2.10) We will discuss the following two systems :

(2.10.1) The Cauchy System : that consisting of any Hamiltonian and Γ_0 a Lagrangian submanifold which is the image (or 'graph') of an exact one-form $-dS_0$, for some scalar valued function S_0 on M , and ,

(2.10.2) The Kernel System : that consisting of any Hamiltonian and Γ_0 a Lagrangian submanifold consisting of the fibre T^*M_q above some point $q \in M$.

(2.11) For these two systems we make the following assumptions :

(2.11.1) <u>The Cauchy Assumption</u> : We assume in the following that the no-caustics condition is satisfied with $I=[0,T]$ for some $T>0$ for the Cauchy System : which will certainly always be the case if for example M is compact or given bounds on S_0 and H and their derivatives . Under this assumption we may define $S:I\times M\to\mathbb{R}$ by :

$S(t,q)=S_0(\pi\theta_t\pi_t^{-1}q)+J_t(\pi_t^{-1}q)$

(2.11.2) <u>The Kernel Assumption</u> : We assume in the following that the no-caustics condition is satisfied with $I=(0,T]$ for some $T>0$ for the Kernel System : this unlike the Cauchy Assumption is a restrictive condition : for example with the $\mathbb{K}^\mu$ – Hamiltonian of (2.8) even if it is non-degenerate ; and unlikely except in special circumstances if it may be degenerate e.g. when L is only hypoelliptic (see §3 for a discussion of the additional problem that arises for degenerate systems) . Under this assumption we may define $S:I\times M\to\mathbb{R}$ by :

$S(t,q)=J_t(\pi_t^{-1}q)$.

(2.12) <u>Remark</u>

For a non-degenerate $\mathbb{K}^\mu$ – Hamiltonian as in (2.8) we may give explicit bounds under which the Cauchy Assumption is satisfied as in **Elworthy and Truman** [1](§3: F-J) and **Elworthy , Truman and Watling** [1](§6) .

(2.13) Theorem

Given either of the systems in (2.10) under the assumptions of the corresponding part of (2.11) with the corresponding definitions of S , S solves the Hamilton-Jacobi equation :

$$\frac{\partial}{\partial t} S(t,q) + H(-dS_t(q)) = 0 .$$

Moreover for the Cauchy System we have the initial condition $S(0,q)=S_o(q)$.

Proof

We will prove the theorem for both systems simultaneously : simply read S_o as 0 in the case of the Kernel System .

Firstly observe that for both systems :

(2.13.1) $$\pi^* dS_o + \alpha = 0 \text{ on } T\Gamma_o .$$

Since for the Kernel System we are reading S_o as 0 , $T\Gamma_o$ is vertical and α annihilates the vertical subundle , see (2.2.1) ; and for the Cauchy System $\pi^* dS_o + \alpha = 0$ on Γ_o as for $Z \in TT^*M_p$:

$$\langle(\pi^* dS_o + \alpha)(p), Z(p)\rangle = \langle p_q + dS_o(q), T\pi(Z(p))\rangle ,$$

since if $\pi(p)=q$ and $p \in \Gamma_o$ means that $p_q = -dS_o(q)$.

Then note :

$$dS_t(q) = ((\pi\theta_t \pi_t^{-1})^* dS_o)(q) + ((\pi_t^{-1})^* dJ_t)(q)$$

$$= ((\pi_t^{-1})^* \theta_t^* \pi^* dS_o)(q) + ((\pi_t^{-1})^* \theta_t^* \alpha)(q) - ((\pi_t^{-1})^* \alpha)(q)$$

by (2.6.2) , so :

(2.13.2) $dS_t(q) = -\pi_t^{-1}(q)$,using (2.13.1) and (2.2.2) .

Now :

$$\frac{\partial}{\partial t} S(t,q) = \langle (\pi^* dS_o)(\theta_t \pi_t^{-1} q) , \frac{\partial}{\partial t}\theta_t \pi_t^{-1} q\rangle + \langle dJ_t(\pi_t^{-1}q), \frac{\partial}{\partial t}\pi_t^{-1} q\rangle$$

$$+ \frac{\partial}{\partial s}\Big|_{s=t} J_s(\pi_t^{-1} q)$$

$$= \langle (\pi^* dS_o)(\theta_t \pi_t^{-1} q) , T\theta_t (Z_H(\pi_t^{-1} q) + \frac{\partial}{\partial t}\pi_t^{-1} q)\rangle$$

$$+ \langle (\theta_t^* \alpha - \alpha)(\pi_t^{-1} q) , \frac{\partial}{\partial t}\pi_t^{-1} q\rangle + \langle (\theta_t^* \alpha)(\pi_t^{-1} q) , Z_H(\pi_t^{-1} q)\rangle$$

$$- H(\pi_t^{-1} q)$$

using (2.6.3) (2.6.2) and (2.6.1) ,

$$= \langle (\pi^* dS_o + \alpha)(\theta_t \pi_t^{-1} q) , T\theta_t (Z_H(\pi_t^{-1} q) + \frac{\partial}{\partial t}\pi_t^{-1} q)\rangle$$

$$- \langle \alpha(\pi_t^{-1} q) , \frac{\partial}{\partial t}\pi_t^{-1} q)\rangle - H(\pi_t^{-1} q)$$

$$= - H(-dS_t(q))$$

using (2.13.1) , $\frac{\partial}{\partial t}\pi_t^{-1} q$ is vertical , (2.2.1) and (2.13.2) .

□

(2.14) Remark

In particular the theorem is true for the K^{μ} - Hamiltonian as in (2.8) .

(2.15) Proposition

In the same circumstances as Theorem (2.13) . For $s \geq 0$ and $R:\Gamma_s \to \mathbb{R}$ define $\underline{R}^s : I \times M \to \mathbb{R}$ by : $\underline{R}^s(t,q) = R(\theta_{t-s}\pi_t^{-1}q)$ then :

$$\frac{\partial}{\partial t}\underline{R}^s(t,q) = \langle d\underline{R}_t^s(q), T\pi(Z_H(\pi_t^{-1}q))\rangle$$

Proof

$$\frac{\partial}{\partial t}\underline{R}^s(t,q) = \langle dR(\theta_{t-s}\pi_t^{-1}q), \frac{\partial}{\partial t}\theta_{t-s}\pi_t^{-1}q\rangle$$

$$= \langle dR(\theta_{t-s}\pi_t^{-1}q), T\theta_{t-s}(Z_H(\pi_t^{-1}q) + \frac{\partial}{\partial t}\pi_t^{-1}q)\rangle$$

using (2.6.3) ,

$$= \langle d\underline{R}_t^s(q), T\pi(Z_H(\pi_t^{-1}q))\rangle$$

as π_t is a diffeomorphism and $\frac{\partial}{\partial t}\pi_t^{-1}q$ is vertical .

□

(2.16) Remark

In particular the proposition is true for the K^{μ} - Hamiltonian as in (2.8) .

§3 The Classical Mechanics Associated with a Semi-Elliptic Differential Operator on a Manifold

(3.0) In (2.8) we defined the K^μ- Hamiltonian governing the Hamiltonian Classical Mechanics associated with a scalar second order semi-elliptic differential operator K^μ on a manifold M of the form :

$$K^\mu = \mu^2 L + Y + W + \frac{V}{\mu^2},$$

where L is a scalar second order semi-elliptic differential operator, Y is a vector field and W and V are real valued functions .

(3.1) Definition

The Lagrangian corresponding with a given Hamiltonian $H:T^*M\to\mathbb{R}$ is a function $L:TM\to\mathbb{R}\cup\{+\infty\}$ defined by :

$$L(v) = \sup_{p\in\pi^{-1}(\{q\})} \{ \langle p,v\rangle - H(p)\}, \text{ if } \pi(v)=q .$$

(3.2) Remarks

(3.2.1) The Lagrangian corresponding to a K^μ - Hamiltonian , which we will refer to as a K^μ - Lagrangian , is given by :

$$L(v) = Q_q^*(v_q - Y(q)) - V(q) , \text{ if } \pi(v)=q ,$$

where Q_q^* is the dual of the quadratic form Q_q , i.e. :

$$Q_q^*(w_q) = \sup_{p_q\in T^*M_q} \{ \langle p_q,w_q\rangle - Q_q(p_q) \}, \text{ for } w_q\in TM_q ,$$

$= Q_q(p_q)$ if $\exists p_q \in T^*M_q$ such that $A_q(p_q) = w_q$
and is $+\infty$ otherwise .

Recall that if we view Q^* as a function $Q^*:TM \to [0,+\infty]$ it is lower semi-continuous (see **Azencott** [1]) and therefore L is as well .

(3.2.2) If there exists a smooth $X:M \to L(\mathbb{R}^n,TM)$ such that $A = XX^*$ then we have :

$$Q_q^*(w_q) = \frac{1}{2}|e|^2 \text{ , if } \exists e \in ImX_q^* = (KerX_q)^\perp \text{ s.t. } X_q(e) = w_q \in TM_q \text{ ,}$$
and is $+\infty$ otherwise .

$$= \inf \{ \tfrac{1}{2}|e|^2 \mid e \in R^n \text{ and } X_q(e) = w_q \} .$$

with the usual convention that $\inf \emptyset = +\infty$.

(3.2.3) If L is elliptic then : $Q^*(v) = \frac{1}{2}\|v\|^2$, where $\|.\|$ is the Riemannian norm associated with L as in (1.6.1) . Thus :

$$L(v) = \tfrac{1}{2}\| v_q - Y(q) \|^2 - V(q) \text{ , if } \pi(v) = q \text{ .}$$

<u>From now on we retrict attention to K^* - Hamiltonians and their associated K^* - Lagrangians .</u>

(3.3) <u>Definition</u>

The Action corresponding to either the Kernel System (2.10.2) or the Cauchy System (2.10.1) of an absolutely continuous path $\gamma:[0,t] \to M$ is defined by :

$$S_t(\gamma) = S_0(\gamma(t)) + \int_0^t L(\gamma'(s))\, ds \text{ ,}$$

if γ is continuous but not absolutely we take it's action to be $+\infty$.

We continue to follow the convention of §2 that if we are discussing the Kernel System we read S_e as 0 , otherwise S_e is the function giving rise to Γ_e in the Cauchy System .

Now if for example S_e is bounded below and V is bounded above then $S_t : C([0,t],M) \to \mathbb{R}\cup\{+\infty\}$ is lower semi-continuous and has the property that $\{ \gamma \mid S_t(\gamma) \leq a\}$ is compact for all $a \in \mathbb{R}$ (a minor extension of **Azencott** [1]) . We assume in the following that S_t is l.s.c. with this compactness property .

(3.4) Remark

In the study of Large Deviations of Diffusion Processes the action in the case $\mathbb{L} = \mathbb{L}_e$, Y=0 , W=V=0 and S_e=0 (particularly for the Kernel System) is often called the Cramer Transform of the diffusion process .

(3.5) Remark

(3.5.1) It is well known in the case that $\mathbb{L}$ is elliptic that we have a correspondence between the K^{μ} - Hamiltonian and K^{μ} - Lagrangian Mechanics as follows : the paths γ that are extremals of the action functional with the boundary conditions $\gamma(0)=q$ and $\gamma(t) \in \Pi\Gamma_e$ are precisely the projections of solutions ρ of Hamilton's Equation with the boundary conditions $\Pi\rho(0)=q$ and $\rho(t) \in \Gamma_e$.

(3.5.2) In fact they are also solutions of the corresponding Newton's Equation :

$$\frac{D^2}{\partial s^2}\Phi(s,q) = -\nabla V(\Phi_s(q)) - Y(\Phi_s(q)),$$

with the boundary conditions $\Phi(0,q)=q$ and $\Phi'(t,q)\in A(\Gamma_o)$, where ∇ denotes the gradient with respect to the natural Riemannian structure induced by an elliptic L as in (1.6) and D denotes the covariant derivative with respect to the Levi-Civita connection of this Riemannian structure .

(3.6) Proposition

If γ is the projection of a solution of Hamilton's Equation ρ then :

$$S_t(\gamma) = S_o(\Pi\rho(t)) + \int_0^t \alpha(Z_H(\rho(s)))-H(\rho(s)) \, ds ,$$

Proof

$\gamma(s) = \Pi\rho(s)$ and $\frac{d}{ds}\rho(s) = Z_H(\rho(s))$, thus $\frac{d}{ds}\gamma(s) = A(\rho(s)) + Y(\gamma(s))$.

So we have :

$$S_t(\gamma) = S_o(\gamma(t)) + \int_0^t Q^*(\gamma'(s) - Y(\gamma(s))) - V(\gamma(s))ds$$

$$= S_o(\gamma(t)) + \int_0^t Q^*(A(\rho(s))) - V(\gamma(s))ds$$

$$= S_e(\gamma(t)) + \int_0^t Q(\rho(s)) - V(\gamma(s))ds \text{ , by (3.2.1) ,}$$

$$= S_e(\gamma(t)) + \int_0^t \alpha(Z_H(\rho(s))) - H(\rho(s))\, ds \text{ , by (2.8.1) .}$$

□

(3.7) Remark

Thus $S_t(q)$ defined in (2.11) is the action of the projection of the solution of Hamilton's Equation $\rho(s)=\theta_s\pi_t^{-1}q$, i.e. the path $\gamma(s)=\pi\theta_s\pi_t^{-1}q$.

(3.8) Remark

If there exists a solution of Hamilton's Equation satisfying the boundary conditions $\pi\rho(0)=q$ and $\rho(t)\epsilon\Gamma_e$ then its projection γ can be seen to be an extremal of the action over paths subject to the boundary conditions $\gamma(0)=q$ and $\gamma(t)\epsilon\pi\Gamma_e$: but in general not every extremal of the action will arise in this way , see **Gaveau** [1] & [2] and **Azencott et al** [1] .

For the rest of this section we assume that there exists a smooth $X:M\to L(\mathbb{R}^n,TM)$ such that $A=XX^*$.

(3.9) For $t>0$ let $H_t=L^2([0,t];\mathbb{R}^n)$ and for $h\epsilon H_t$ consider the ordinary differential equation :

$$\frac{d}{ds}\varphi(s,h,q) = X(\varphi(s,h,q))(h(s)) + Y(\varphi(s,h,q)) \text{ ,}$$

$\varphi(0,h,q) = q$

(3.10) Proposition

Assuming non-explosion of the solutions of (3.9) before time t which we assume in all that follows, which certainly will be the case when M is compact or given bounds on the derivatives of X and Y, $\varphi(s,h,.):M\to M$ is a flow of smooth diffeomorphisms depending continuously on $s\in[0,t]$.

$\varphi(s,.,q):H_t\to M$ is smooth for each $s\in[0,t]$ and $q\in M$ with

$\frac{d}{dh}\varphi(s,h,q):H_t\to L(H;TM_{\varphi(s,h,q)})$ given by :

$$\frac{d}{dh}\varphi(s,h,q)(k) = T\varphi(s,h,.)(q)\int_0^s (\varphi(r,h,.)^{*^{-1}}X)(q)(k(r))\,dr$$

$$= T\varphi(s,h,.)(q)\int_0^s \sum_{i=1}^n(\varphi(r,h,.)^{*^{-1}}X_i)(q)\,k_i(r)\,dr$$

where X_i is given by some orthonormal basis of R^n as in (1.13).

Proof

Standard results plus elementary calculation.

□

(3.11) Definition

The 'Deterministic Malliavin Covariance Matrix' associated with $\varphi(s,h,q)$ is a map $C(s,h):M\to L(T^*M,TM)\cong TM\otimes TM$ for $s\in[0,t]$ and $h\in H_t$ defined by :

$$C(s,h)(q) = \int_0^s (\varphi(r,h,.)^{*^{-1}} A)(q)\, dr$$

$$= \int_0^s (\varphi(r,h,.)^{*^{-1}} X)(q)\, (\varphi(r,h,.)^{*^{-1}} X^*)(q)\, dr$$

So for $p_q \varepsilon T^* M_q$:

$$C(s,h)(q)(p_q) = \int_0^s \sum_{i=1}^n \langle p_q , (\varphi(r,h,.)^{*^{-1}} X_i)(q) \rangle (\varphi(r,h,.)^{*^{-1}} X_i)(q)\, dr$$

(3.12) Remark

The reason we have called this the 'Deterministic Malliavin Covariance Matrix' is that when the above equation (3.9) is relaced by a Stratonovich stochastic differential equation (formally replace h(s) by $\frac{d\omega}{ds}(s)$ where $\omega(s)$ is n-dimensional Brownian Motion and rewrite in the standard integral way for Stochastic differential equations) then $\varphi(s,\omega,.)$ becomes the stochastic flow and $C(s,\omega)$ the usual Malliavin Covariance Matrix . This terminology is due to **Bismut** [1] .

(3.13) Proposition

$C(s,h)(q)$ is invertible if and only if $\frac{d}{dh}\varphi(s,h,q)$ is surjective .

Proof

$$\frac{d}{dh}\varphi(s,h,q) \{ \frac{d}{dh}\varphi(s,h,q) \}^* = T\varphi(s,h,.)(q) C(s,h)(q) \{ T\varphi(s,h,.)(q) \}^*$$

This expression will occur later in (3.23) and in §8 so we call it $K(s,h)(q)$, this is in $L(T^*M_{\psi(s,h,q)},TM_{\psi(s,h,q)})$.

□

(3.14) Proposition

If $Z:M\to L(\mathbb{R}^m;TM)$ satisfies $A=ZZ^*$ then $\exists k\in K_t=L^2([0,t];\mathbb{R}^m)$ such that $\varphi(s,h,q)=\psi(s,k,q)$ $\forall s\in[0,t]$, where $\psi(s,k,q)$ is the solution of the differential equation corresponding to the Z decomposition of A . Moreover $C(s,h)(q)$ is invertible if and only if the corresponding $D(s,k)(q)$ is invertible , where $D(s,k)(q)$ is the 'Deterministic Malliavin Covarince Matrix' corresponding to $\psi(s,k,q)$. Thus invertibility of the 'Deterministic Malliavin Covarince Matrix' is a property of the pair (L,Y) and does not depend on which decomposition of A is chosen .

Proof

Take orthonormal bases of $\mathbb{R}^n$ and $\mathbb{R}^m$ and let X_i and Z_j for $1\le i\le n$ and $1\le j\le m$ denote the vector fields associated with X and Z as in (1.13) .

Now for $1\le i\le n$ and $1\le j\le m$ there exist smooth functions $\lambda_i^j:M\to\mathbb{R}$ such that :

$$X_i=\sum_{j=1}^{m}\lambda_i^j Z_j .$$

So given $h \in H_t$ let $k \in K_t$ be given by :

$$k^j(s) = \sum_{i=1}^{n} \lambda_i^j(\varphi(s,h,q))h^i(s) \text{ , for } 1 \le j \le m \text{ .}$$

Then clearly $\psi(s,k,q)=\varphi(s,h,q)$ for all $s \in [0,t]$, since both solve :

$$\frac{d}{ds}\psi(s,k,q) = Z(\psi(s,k,q))(k(s)) + Y(\psi(s,k,q)) \text{ ,}$$

$$\text{for } Z(\psi(s,k,q))(k(s)) = \sum_{j=1}^{m} Z_j(\psi(s,k,q))k^j(s)$$

$$= \sum_{j=1}^{m} Z_j(\psi(s,k,q)) \sum_{i=1}^{n} \lambda_i^j(\varphi(s,h,q))h^i(s)$$

$$= \sum_{i=1}^{n} \{ \sum_{j=1}^{m} \lambda_i^j(\varphi(s,h,q))Z_j(\psi(s,k,q)) \} h^i(s) \text{ .}$$

We give a local argument to show that $\frac{\partial\psi}{\partial k}(s,k,q)$ and $\frac{\partial\varphi}{\partial h}(s,h,q)$ have the same images for all $s \in [0,t]$, whence (3.13) gives us : $C(s,h)(q)$ is invertible if and only if $D(s,k)(q)$ is invertible .

Let $x(s)$ be the coordinates of $\varphi(s,h,q) = \psi(s,k,q)$ in a chart as in (2.1) , and let $u \in H_t$ then $U(s) = \frac{\partial\varphi}{\partial h}(s,h,q)(u)$ solves the following equation :

$$\frac{dU^i}{ds}(s) = \sum_{k=1}^{n} \{ \sum_{j=1}^{d} \frac{\partial X_k^i}{\partial x^j}(x(s))U^j(s)h^k(s) + X_k^i(x(s))u^k(s) \} + \sum_{j=1}^{d} \frac{\partial Y^i}{\partial x^j}(x(s))U^j(s)$$

$U^i(0) = 0$

where superscripts denote components in our chart .

$$\text{But } \frac{\partial X_k^i}{\partial x^j}(x(s)) = \sum_{l=1}^{m} \{ \frac{\partial \lambda_k^l}{\partial x^j}(x(s)) Z_l^i(x(s)) + \lambda_k^l(x(s)) \frac{\partial Z_l^i}{\partial x^j}(x(s)) \}$$

So :

$$dU^i(s) = \sum_{l=1}^{m} \{ \sum_{j=1}^{d} \frac{\partial Z_l^i}{\partial x^j}(x(s)) U^j(s) k^l(s) ds$$

$$+ Z_l^i(x(s)) \sum_{k=1}^{n} [\sum_{j=1}^{d} \frac{\partial \lambda_k^l}{\partial x^j}(x(s)) U^j(s) h^k(s) + \lambda_k^l(x(s)) u^k(s)] \}$$

$$+ \sum_{j=1}^{d} \frac{\partial Y^i}{\partial x^j}(x(s)) U^j(s)$$

So taking $v^l(s) = \sum_{k=1}^{n} [\sum_{j=1}^{d} \frac{\partial \lambda_k^l}{\partial x^j}(x(s)) U^j(s) h^k(s) + \lambda_k^l(x(s)) u^k(s)]$,

we see that $\frac{\partial \psi}{\partial k}(s,k,q)(v) = \frac{\partial \varphi}{\partial h}(s,h,q)(u)$, since both solve :

$$\frac{dV^i}{ds}(s) = \sum_{l=1}^{m} \{ \sum_{j=1}^{d} \frac{\partial Z_l^i}{\partial x^j}(x(s)) V^j(s) k^l(s) + Z_l^i(x(s)) v^l(s) \} + \sum_{j=1}^{d} \frac{\partial Y^i}{\partial x^j}(x(s)) V^j(s)$$

$V^i(0) = 0$

□

(3.15) Definitions

We define the following conditions on the pair (L,Y) at a point $q \in M$:

(H1) $\mathrm{Lie}\{\, X_i \mid 1 \le i \le n \,\}(q) = TM_q$.

(H2) $\mathrm{Lie}\{\, X_i\, ,\, [X_i, Y] \mid 1 \le i \le n \,\}(q) = TM_q$.

(H3) $\forall e \in \{ e \in \mathbb{R}^n \mid X(q)(e) + Y(q) \neq 0 \}$:

$\mathrm{span}\{X_i\, ,\, [X(e)+Y, X_i]\, ,\, [X(e)+Y, [X(e)+Y, X_i]]\, , \ldots\, \}(q) = TM_q$.

It should be noted that (H1) , (H2), and (H3) do not depend on the choice of orthonormal basis or even on the choice of X such that $A = XX^*$, so they are indeed properties of the pair (L,Y) .

(3.16) Proposition

(i) If L is elliptic at q then then $C(s,h)(q)$ is invertible for all $h \in H_t$ and $s \in (0,t]$.

(ii) If L satisfies (H3) at q then $C(t,h)(q)$ is invertible for all $h \notin L^2([0,t],E)$, where E is the closed affine subspace $X(q)^{-1}(\{-Y(q)\})$.

(3.17) Remark

If the pair (L,Y) only satisfy (H1) or (H2) at q then we may only deduce that $C(s,h)(q)$ is invertible for all $h \in H_t$ in a weakly dense set and $s \in (0,t]$, see Bismut [1] to get an idea of the proof of this from the Malliavin Calculus . This will be seen to be insufficient for our purposes of relating extremals of the action functional with projections of solutions to the corresponding Hamilton's Equation .

<u>Proof of (3.16)</u>

(i) L elliptic at q means that $A(q)$ is invertible and hence so is $C(s,h)(q)$ for all $h\in H_1$ and $s\in(0,t]$.

(ii) By shifting time we may as well assume that h almost surely does not take values in E on some interval $[0,\varepsilon]$ where $\varepsilon>0$, that is for almost all $s\in[0,\varepsilon]$ $X(q)(h(s)) + Y(q) \neq 0$.

Let $p_q\in T^*M_q$ satisfy $C(t,h)(q)(p_q)=0$, then :

$$(3.16.1)\quad 0=\langle p_q\,,\,C(t,h)(q)(p_q)\rangle = \int_0^t \sum_{i=1}^n \langle p_q\,,\,((\varphi(s,h,.)^{*})^{-1}X_i)(q)\rangle^2\, ds\,.$$

So for all $1\le i\le n$ and $s\in[0,t]$:

$$(3.16.2)\quad \langle p_q\,,\,((\varphi(s,h,.)^{*})^{-1}X_i)(q)\rangle = 0\,.$$

Now by definition of the Lie derivative of a vector field Z on M :

$$((\varphi(s,h,.)^{*})^{-1}Z)(q) = Z(q) + \int_0^s ((\varphi(r,h,.)^{*})^{-1}[X(h(r))+Y,Z])(q)\, dr\,.$$

Letting $Z=X_i$ and substituting in (3.16.1) and using (3.16.2) we deduce that for all $1\le i\le n$ and $s\in[0,t]$:

$$\langle p_q\,,\,\int_0^s ((\varphi(r,h,.)^{*})^{-1}[X(h(r))+Y,X_i])(q)dr\rangle = 0\,.$$

Whence for all $1\le i\le n$ and almost all $s\in[0,t]$:

$$\langle p_q\,,\,((\varphi(s,h,.)^{*})^{-1}[X(h(r))+Y,X_i])(q)dr\rangle = 0\,.$$

Continuing in this way we deduce that for all $1 \le i \le n$, almost all $s \in [0,t]$ and any number of Lie brackets :

$$\langle p_q , (\varphi(s,h,.)^*)^{-1}[X(h(r))+Y,[X(e)+Y,[....[X(e)+Y,X_i]....]]])(q)dr\rangle = 0 .$$

Now $(\varphi(s,h,.)^*)^{-1}$ of the vector fields appearing in (H3) i.e. $[X(e)+Y,[X(e)+Y,[....[X(e)+Y,X_i]....]]]$ will still span TM_q and for almost all $r \in [0,\varepsilon]$ $X(q)(h(r))+Y(q) \neq 0$, thus we conclude $p_q = 0$ and $C(t,h)(q)$ is invertible .

□

(3.18) <u>Definition</u>

Let $I_t : H_t \to \mathbb{R}$ be defined by :

$$I_t(h) = S_e(\varphi(t,h,q)) + \int_0^t \tfrac{1}{2}|h(s)|^2 - V(\varphi(s,h,q))\, ds$$

with the same convention as in (3.3) that if we are investigating the kernel system we read S_e as zero .

(3.19) <u>Notation and Remarks</u>

Let $\Lambda(q,\Gamma_e,t) = \{\gamma:[0,t] \to M \text{ continuous} \mid \gamma(0)=q , \gamma(t) \in \Pi\Gamma_e \}$

and $K(q,\Gamma_e,t) = \{h \in H_t \mid \varphi(t,h,q) \in \Pi\Gamma_e \}$.

Then $E(q,\Gamma_e,t) = \inf_{h \in K(q,\Gamma_e,t)} I_t(h) = \inf_{\gamma \in \Lambda(q,\Gamma_e,t)} S_t(\gamma)$.

For the Kernel System it is known that if $K(q,\Gamma_e,t) \neq \emptyset$ then there exists $h \in K(q,\Gamma_e,t)$ such that $I_t(h) = E(q,\Gamma_e,t)$ from l.s.c and compactness as in (3.3). Moreover if L satisfies (H1) at every $q \in M$ then $K(q,\Gamma_{*},t) \neq \emptyset$.

(3.20) <u>Proposition</u>

If $p \in T^{*}M$ with $\pi(p)=q$ and we define $h(s)=X^{*}(\theta_s(p))$, where θ is the flow corresponding to our K^{*} Hamiltonian, then:

$\varphi(s,h,q) = \pi\theta_s(p)$, and

$$\theta_s(p)_{\varphi(s,h,q)} = [T\varphi(s,h,.)(q)^{*}]^{-1}\{ p_q - \int_0^s d(V\circ\varphi(r,h,.))(q)\,dr\}.$$

<u>Proof</u>

$$\frac{d}{ds}\varphi(s,h,q) = X(\varphi(s,h,q))(h(s)) + Y(\varphi(s,h,q))$$

$$= X(\varphi(s,h,q))(X^{*}(\theta_s(p))) + Y(\varphi(s,h,q))$$

So since $\pi\theta_s(p)$ is clearly a solution with $\pi\theta_0(p) = q$ we deduce the first part.

We will give a local argument below to show that

$v(s) = T\varphi(s,h,.)(q)^{*}(\theta_s(p)_{\varphi(s,h,q)})$

is the solution of the following differential equation in $T^{*}M_q$:

$$\frac{d}{ds}v(s) = -d(V\circ\varphi(s,h,.))(q)$$

with initial condition $v(0) = p_q$. Whence the result follows as:

$p_q - \int_0^s d(V\circ\varphi(r,h,.))(q)\,dr$, is clearly the solution.

Let $(y(s),x(s))$ be the coordinates of $\theta_s(p)$ in a chart as in (2.1) then :

$$\frac{dx^j(s)}{ds} = \sum_{k=1}^{n} X_k^j(x(s))h^k(s) + Y^j(x(s)) ,$$

where X_k^j and Y^j are the jth components of the vector fields X_k and Y in our coordinate system and :

$$h^k(s) = \sum_{k=1}^{n} X_k^m(x(s))y_m(s) .$$

Thus :

$$\frac{d}{ds}\frac{\partial x^j(s)}{\partial x^i} = \sum_{k=1}^{d}\Big\{ \sum_{l=1}^{n} \frac{\partial X_k^j(x(s))}{\partial x^l}\frac{\partial x^l(s)}{\partial x^i} h^k(s) + \frac{\partial Y^j(x(s))}{\partial x^l}\frac{\partial x^l(s)}{\partial x^i} \Big\}$$

So :

$$\frac{d v^i(s)}{ds} = \sum_{j=1}^{d} \frac{d}{ds}\Big\{ \frac{\partial x^j(s)}{\partial x^i} y_j(s) \Big\}$$

$$= \sum_{j=1}^{d}\Big\{ y_j(s)\frac{d}{ds}\frac{\partial x^j(s)}{\partial x^i} + \frac{\partial x^j(s)}{\partial x^i}\frac{d y_j(s)}{ds} \Big\}$$

$$= \sum_{j,l=1}^{d}\sum_{m=1}^{n} \Big[y_j(s)y_m(s)\frac{\partial x^l(s)}{\partial x^i}\Big(\sum_{k=1}^{n}\frac{\partial X_k^j(x(s))}{\partial x^l} X_k^m(x(s)) - \frac{1}{2}\frac{\partial a_{jm}(x(s))}{\partial x^l} \Big)\Big]$$

$$- \sum_{j=1}^{d}\frac{\partial x^j(s)}{\partial x^i}\frac{\partial V(x(s))}{\partial x^j} .$$

But :

$$a_{jm} = \sum_{k=1}^{n} X_k^j X_k^m \text{ so } \frac{\partial}{\partial x^l} a_{jm} = 2 \sum_{k=1}^{n} X_k^m \frac{\partial}{\partial x^l} X_k^j .$$

Thus $v(s)$ solves the required equation .

□

(3.21) Theorem

(i) For the Kernel System if $K(q,\Gamma_*,t) \neq \emptyset$ (so in particular if L satisfies (H1) at all $q \in M$)and $h \in K(q,\Gamma_*,t)$ satisfies $I_t(h) = E(q,\Gamma_*,t)$ and $C(t,h)(q)$ is invertible (so in particular this is true if (L,Y) satisfies (H3) at q and if L is not elliptic at q and $\pi\Gamma_* = \{q\}$ that $h \notin L^2([0,t],E)$) , then there exists a unique $p \in T^*M$ such that $\varphi(s,h,q) = \pi\theta_s(p)$ for all $s \in [0,t]$.

(ii) For the Cauchy System if $h \in H_t$ satisfies $I_t(h) = E(q,\Gamma_*,t)$ then there exists $p \in T^*M$ such that $\varphi(s,h,q) = \pi\theta_s(p)$ for all $s \in [0,t]$ (this p is unique if $C(t,h)(q)$ is invertible - so in particular this is true if (L,Y) satisfies (H3) at q and if L is not elliptic at q that $h \notin L^2([0,t],E)$) .

Proof

(i) As $C(t,h)$ is invertible $K(q,\Gamma_*,t)$ is a submanifold of H_t in a neighbourhood of h .

As h is a minimum of I_t on $K(q,\Gamma_*,t)$ we have $dI_t(h) = 0$, so for all $v \in T_hK(q,\Gamma_*,t)$ we have :

$$0 = \langle dI_t(h), v\rangle = \langle h,v\rangle - \int_0^t \langle dV(\varphi(s,h,q)), \frac{d}{dh}\varphi(s,h,q)(v)\rangle ds$$

$$= \langle h,v\rangle - \int_0^t \langle d(V\circ\varphi(s,h,.))(q), \int_0^s (\varphi(r,h,.)^{*-1} X)(q)(v(r))dr\rangle ds$$

$$= \langle h(r) - (\varphi(r,h,.)^{*-1} X^*)(q)\int_r^t d(V\circ\varphi(s,h,.))(q)ds \, , \, v(r)\rangle$$

Thus $h(r) - (\varphi(r,h,.)^{*-1} X^*)(q)\int_r^t d(V\circ\varphi(s,h,.))(q)ds \in T_h K(q,\Gamma_\bullet,t)^\perp$.

But :

$$v \in T_h K(q,\Gamma_\bullet,t) \Leftrightarrow \int_0^t (\varphi(s,h,.)^{*-1} X)(q)(v(s))ds = 0$$

and :

$w(r) \in T_h K(q,\Gamma_\bullet,t)^\perp \Leftrightarrow \exists p_q \in T^*M_q$ such that $w(r) = (\varphi(r,h,.)^{*-1} X^*)(q)(p_q)$.

This p_q is in fact unique as :

$$0 = \|(\varphi(r,h,.)^{*-1} X^*)(q)(p_q)\|^2 = \langle p_q, C(t,h)(q)(p_q)\rangle \Rightarrow p_q = 0 \, ,$$

means that the linear map from T^*M_q to H_t defined by :

$$p_q \to (\varphi(r,h,.)^{*-1} X^*)(q)(p_q) \, ,$$

is injective . Observe that $T_h K(q,\Gamma_\bullet,t)$ is the kernel of the adjoint of this linear map and that $T_h K(q,\Gamma_\bullet,t)^\perp$ is its image .

So we conclude that there exists a unique $p'_q \in T^*M_q$ such that for almost all $r\in[0,t]$:

$$h(r) = (\varphi(r,h,.)^{*^{-1}} X^*)(q)\{\, p'_q + \int_r^t d(V o\varphi(s,h,.))(q)ds \,\}$$

So if we let $p_q = p'_q + \int_r^t d(V o\varphi(s,h,.))(q)ds$ then :

$$h(r) = X^*\{\, [T\varphi(r,h,.)(q)^*]^{-1} (p_q - \int_0^r d(V o\varphi(s,h,.))(q)ds \,\}$$

So from (3.20) we deduce that $\Pi\theta_s(p) = \varphi(s,h,q)$.

(ii) We have $K(q,\Gamma_e,t) = H_t$. As h is a minimum of I_t on H_t we have in a similar way to part (i) that for all $v\in H_t$:

$$0 = \langle h(r) + (\varphi(r,h,.)^{*^{-1}} X^*)(q)\{d(S_e o\varphi(t,h,.))(q) - \int_r^t d(V o\varphi(s,h,.))(q)ds\}, v(r)\rangle$$

Thus $h(r) = (\varphi(r,h,.)^{*^{-1}} X^*)(q)\{\, -d(S_e o\varphi(t,h,.))(q) + \int_r^t d(V o\varphi(s,h,.))(q)ds \,\}$

So if we let $p_q = -d(S_e o\varphi(t,h,.))(q) + \int_r^t d(V o\varphi(s,h,.))(q)ds$, we have :

$$h(r) = X^*\{\, [T\varphi(r,h,.)(q)^*]^{-1} (p_q - \int_0^r d(V o\varphi(s,h,.))(q)ds \,\}$$

So from (3.20) we deduce that $\pi\theta_s(p) = \varphi(s,h,q)$.

p_q must be unique if $C(t,h)(q)$ is invertible due to the injectivity of the linear map in part (i) .

□

(3.22) Remark

(3.22.1) We have assumed a no caustics assumption for the Cauchy System in (2.11.1) so provided $t \le T$ there is only one p which can give a minimum and thus we do not need to worry about non-uniqueness of p for given h as there is only one possible p .

(3.22.2) We need some such condition as invertibility of $C(t,h)(q)$ for the Kernel System because Gaveau (see **Gaveau** [1] & [2] and **Azencott et al** [1]) has examples of natural operators on rank 2 Nilpotent groups satisfying (H1) , so there exists a minimising h , but the corresponding path is not realised as a projection of a solution of the associated Hamilton's Equation .

(3.23) Proposition

For the Kernel System of (2.10.2) with $\Gamma_s = T^*M_y$ under the no Caustics Assumption of (2.11.2) for a K^μ – Hamiltonian with V=0 and $C(t,h)(q)$, or equivalently $K(t,h)(q)$ of (3.13) , invertible for h given by $h(s) = X^*(\theta_s \pi_t^{-1} q)$ we have :

$$S_t(q) = \tfrac{1}{2}\langle \Pi_t^{-1}q, C(t,h)(q)(\Pi_t^{-1}q)\rangle$$

$$= \tfrac{1}{2}\langle K(t,h)(q)^{-1}(v_t(q)), v_t(q)\rangle ,$$

where $v_t(q) = K(t,h)(q)(\theta_t\Pi_t^{-1}q)\epsilon TM_y$.

<u>Proof</u>

$$S_t(q) = \frac{1}{2}\int_0^t Q(\theta_s\Pi_t^{-1}q)\, ds ,$$

$$= \frac{1}{2}\int_0^t \langle \theta_s\Pi_t^{-1}q, A(\theta_s\Pi_t^{-1}q)\rangle\, ds ,$$

$$= \frac{1}{2}\int_0^t \langle [T\varphi(s,h,.)(q)^*]^{-1}(\Pi_t^{-1}q), A([T\varphi(s,h,.)(q)^*]^{-1}(\Pi_t^{-1}q))\rangle\, ds ,$$

by (3.20) ,

$$= \frac{1}{2}\int_0^t \langle \Pi_t^{-1}q, (\varphi(s,h,.)(q)^{*^{-1}} A)(\Pi_t^{-1}q)\rangle\, ds ,$$

$$= \tfrac{1}{2}\langle \Pi_t^{-1}q, C(t,h)(q)(\Pi_t^{-1}q)\rangle ,$$

by definition of $C(t,h)(q)$,

$$= \tfrac{1}{2}\langle K(t,h)(q)^{-1}(v_t(q)), v_t(q)\rangle ,$$

by definition of $K(t,h)(q)$ and $v_t(q)$.

□

§4 A First Look at Some Semi-Classical Semigroups

(4.0) Assumptions

(4.0.1) Regularity Assumption : We suppose that there exists a semigroup $P^{\mu}(t)$ with infinitesimal generator K^{μ} on smooth functions of compact support , which preserve smooth functions : which will certainly be the case if L is elliptic or L is hypoelliptic and we are given appropriate bounds on the coefficients of K^{μ} and their derivatives .

(4.0.2) No Caustics Assumption : We suppose we are in the situation of Theorem (2.13) for the K^{μ} - Hamiltonian .

(4.1) In the situation of (4.0) , define the operators :

$$\{Q^{\mu}(t,r)g\}(q)=\exp\left(\frac{S(t,q)}{\mu^2}\right)\{P^{\mu}(t-r)\exp\left(\frac{-S_r}{\mu^2}\right)g\}(q)\text{ , for } t,r\in I \text{ with } r\le t \text{ ,}$$

on scalar valued functions g on M for which the right hand side is defined : which will certainly include smooth g of compact support .

(4.2) Lemma

Formally these operators form a time inhomogenous semi-group i.e. : $Q^{\mu}(t,s)\,Q^{\mu}(s,r)=Q^{\mu}(t,r)$, for $r,s,t\in I$ with $r\le s\le t$,and moreover for smooth g of compact support we have :

(4.2.1) $$\frac{\partial}{\partial t}\{Q^{\mu}(t,r)g\}(q)=\{I(t)Q^{\mu}(t,r)g\}(q)\text{ , for } r,t\in I \text{ with } r\le t$$

(4.2.2) $$\frac{\partial}{\partial r}\{Q^{\mu}(t,t-r)g\}(q)=\{Q^{\mu}(t,t-r)\,I(t-r)\,g\}(q)\text{ , for } r,t-r\in I \text{ with } r\ge 0$$

Where $I(s)$ for $s \in I$ is the time dependent smooth scalar second order semi-elliptic differential operator $\mu^2 L + (Y - A(dS_s)) + (W - L_o S_s)$.

Proof

(4.2.1) For any smooth h of compact support we have :

$$\frac{\partial}{\partial t} \exp\left(\frac{S(t,q)}{\mu^2}\right)(P^{\mu}(t-r)h)(q) = \exp\left(\frac{S(t,q)}{\mu^2}\right)\left(\left[\frac{\partial}{\partial t}\left(\frac{S_t}{\mu^2}\right) + K^{\mu}\right] P^{\mu}(t-r)h\right)(q)$$

For any smooth k and l we have the commutator :

$$\left[K^{\mu}, \exp\left(\frac{k}{\mu^2}\right) \right](l) = \left(A(dk) + \left(L_o(k) - \frac{Q(dk)}{\mu^2} + \frac{\langle dk, Y\rangle}{\mu^2}\right)\right)\left(\exp\left(\frac{k}{\mu^2}\right) l\right)$$

$$(4.2.3) \qquad = \exp\left(\frac{k}{\mu^2}\right)\left(A(dk) + \left(L_o(k) + \frac{Q(dk)}{\mu^2} + \frac{\langle dk, Y\rangle}{\mu^2}\right)\right)(l)$$

So the result follows from taking :

$h = \exp\left(-\frac{S_r}{\mu^2}\right)g$, $k = S_t$, $l = P^{\mu}(t-r)h$

and applying (2.13) .

(4.2.2) We have :

$$\frac{\partial}{\partial r} P^{\mu}(r)\exp\left(-\frac{S_{t-r}}{\mu^2}\right)g = P^{\mu}(r)\left(\frac{\partial}{\partial r}\left(-\frac{S_{t-r}}{\mu^2}\right) + K^{\mu}\right)\exp\left(-\frac{S_{t-r}}{\mu^2}\right)g$$

So the result follows by taking $k = -S_{t-r}$, $l = g$ in (4.2.3) and applying (2.13) .

Alternatively we could use the semigroup property to prove one from the other , but observe that (4.2.2) does not require P^{μ} to preserve smooth functions .

□

(4.3) Remark

For L any scalar second order differential operator , μ any complex number , P^{μ} any semi-group associated with the corresponding K^{μ} , in the situation of (4.0.2) , (4.2.2) is true , and given that this P^{μ} preserves smooth functions (4.2.1) is true .

(4.4) Theorem

With the assumptions of (4.0) and further assuming $W + \mu^2 U - L_{\bullet} S_u$ is bounded above uniformly in u over any compact subinterval of I (which is certainly true for M compact) we have for smooth g of compact support and for $t-r, t \in I$ with $r \geq 0$:

$$\{Q^{\mu}(t,t-r)g\}(q) = E[g(x^{t,\mu}(r)\exp\{\int_0^r (W + \mu^2 U - L_{\bullet} S_{t-u})(x^{t,\mu}(u))du\}] ,$$

where $x^{t,\mu}(\ .\ )$ is the solution of the following stochastic differential equation that we assume to be non-explosive , as will certainly be the case given some bounds or if M is compact : If L is elliptic or we have some other reason to make a natural choice of connection then we will take it to mean an Itô equation with $X_{\bullet} = X_{\bullet}(\nabla)$ as in (1.8) and X as in (1.10) : If we can choose a smooth X then we will take it to mean a Stratonovich equation with $X_{\bullet}(X)$ as in (1.13) :

$$dx^{t,\mu}(u) = \mu X(x^{t,\mu}(u))dB(u) + [\mu^2 X_{\bullet} + Y - A(dS_{t-u})](x^{t,\mu}(u))du$$

$$x^{t,\mu}(0) = q , \text{ where } B(u) \text{ is Brownian Motion on } \mathbb{R}^n .$$

(4.5) Remarks

(4.5.1) This Theorem enables us to extend the domain of $Q^M(t,s)$ to say bounded measurable functions as the right hand side of the above equality makes sense for such functions . They then form a semigroup on this function space .

(4.5.2)When L is Elliptic we could express $x^{t,M}(u)$ as the projection of the solution of a canonical Stratonovich equation on O(M) as indicated in (1.14) and then the case of this Theorem for the Cauchy System with : $r = t$, $L_s = \frac{1}{2}\Delta$, $Y = 0$ and $W = 0$, will be the 'Elementary Formula A' of **Elworthy and Truman** [2] : the case of the theorem with $r=t$ could indeed have been obtained by use of Feynman-Kac-Girsanov transformations as in this reference however the semi-classical semigroup approach makes the iteration process in the next chapter easier to see and clarifies the similarities with the semi-classical analysis of the Schrödinger equation as in **Elworthy and Truman** [1] and **Elworthy , Truman and Watling** [1] . See also (4.9) - (4.11) .

Proof of (4.4)

Define $h : [t-r,t]\times M\times \mathbb{R}\to\mathbb{R}$ by : $h(u,q,v)=v\{Q^M(u,t-r)g\}(q)$, then :

(4.4.1) $\frac{\partial}{\partial u} h(u,q,v) = \{I(u)h(u,v)\}(q)$, by (4.2.1) .

Consider the Process $y^{t,M}(u) = (\tau^t(u)\ ,\ x^{t,M}(u)\ ,\ v^{t,M}(u))$ on the domain of h given by the stochastic differential equation :

$$dx^{t,\mu}(u) = \mu X(x^{t,\mu}(u))dB(u) + [\mu^2 X_0 + Y - A(dS(\tau^t(u)))](x^{t,\mu}(u))du$$

$$d\tau^t(u) = -du$$

$$dv^{t,\mu}(u) = [\mu^2 U - W - L_0 S(\tau^t(u))](x^{t,\mu}(u))v^{t,\mu}(u)du$$

with : $x^{t,\mu}(0) = q$, $\tau^t(0) = t$, $v^{t,\mu}(0) = 1$.

So $\tau^t(u) = t-u$ and $v^{t,\mu}(u) = \exp\{\int_0^u (W + \mu^2 U - L_0 S_{t-s})(x^{t,\mu}(s))ds\}$

and the result follows by applying Itô's Formula to $h(y^{t,\mu}(r))$ applying (4.4.1) to get :

$$v^{t,\mu}(u)g(x^{t,\mu}(u)) = \{Q^\mu(t,t-r)g\}(q) + M(u) ,$$

where $M(u)$ is a martingale with $M(0)=0$, which is bounded as the other non-constant term in the above expression is by assumption . Thus the result follows by taking expectations .

□

(4.6) Remark

This theorem certainly uses the facts that μ is real , L is semi-elliptic and that P^μ preserves smooth functions .

(4.7) Aside

If $M = \mathbb{R}^d$ then we could make use of the ideas of Doss [1] and [2] to obtain a probabalistic representation for $Q^\mu(t,t-r)$ in the case : $\mu^2 = i\hbar$, L given in Hörmander form as in (1.11) and K^μ with an 'analytic extension' to appropriate subsets of $\mathbb{C}^d$. However putting these ideas in a manifold context is not so clear : given a real-analytic structure on M we can construct a natural complexification of M , see **Eastwood** [1] , for which the concept of analytic extension is meaningful and so we have the required complex linearity for the trick, but we still have a choice of real-analytic structure (even on $\mathbb{R}^d$) and so we must ask whether we can find a real-analytic structure on M with respect to which K^μ has an analytic extension to the associated complexification of M .

(4.8) <u>Corollary</u>

Under the same assumptions as the theorem when $\mu \to 0$:

$\{Q^\mu(t,t-r)g\}(q) \to \{M(t,t-r)g\}(q)$,

where for $t,s \in I$:

$\{M(t,s)g\}(q) = g(\pi\theta_{t-s}\pi_t^{-1}q)\varphi(t,s)(q)$,

with :

$$\varphi(t,s)(q) = \exp\{\int_0^{t-s} (W - L_a S_{t-u})(\pi\theta_u\pi_t^{-1}q)du\} .$$

Moreover it is clear that these operators $M(t,s)$ are invertible and form a time inhomogenous semigroup i.e. : $M(t,s)M(s,r) = M(t,r)$, for all t , s and $r \in I$.

<u>Proof</u>

As in **Elworthy and Truman** [2] we can use dominated convergence and the fact that $x^{t,\mu}$ tends uniformly in $u \in [0,r]$ in probability to the solution of :

$dx^{t,\omega}(u) = [Y - A(dS_{t-u})](x^{t,\omega}(u))du$, with $x^{t,\omega}(u) = q$, which is $\pi\theta_u\pi_t^{-1}q$.

□

(4.9) Remarks

(4.9.1) If L is elliptic then as explained in (1.7),(1.8) and (1.9) ,

$$L = \tfrac{1}{2}\Delta + X_o(\nabla) + U .$$

(4.9.2) Also we see from (3.2.3) and (3.7) that :

$$S_t(q) = S_o(\pi\theta_t\pi_t^{-1}q) + \int_0^t \frac{1}{2}\left\| \frac{d}{ds}(\pi\theta_u\pi_t^{-1}q) - Y(\pi\theta_u\pi_t^{-1}q) \right\|^2 - V(\pi\theta_u\pi_t^{-1}q)du$$

where $\|.\|$ is the natural Riemannian norm of (1.6) .

(4.10) Proposition

If L is elliptic then we have for $t,s\in I$:

$$\varphi(t,s)(q) = (\sqrt{\phi(t,s,q)})\exp\{ \int_0^{t-s}(W-X_o(\nabla)(S_{t-u}) - \tfrac{1}{2}\mathrm{div}Y)(\pi\theta_u\pi_t^{-1}q)du \}$$

where $\phi(t,s,q) = |\det T_q(\pi\theta_{t-s}\pi_t^{-1})|$, where the determinant is computed using orthonormal bases of the tangent spaces with respect the natural Riemannian inner product .

(4.11) Remark

If $L_o = \tfrac{1}{2}\Delta$ and $W = \tfrac{1}{2}\mathrm{div}Y$, then $\varphi(t,r)$ is simply the square root of the determinant of the derivative of the time inhomogenous classical flow on M , c.f. the Schrödinger equation in a magnetic field , for example in **Elworthy**, **Truman and Watling** [1] where : $\mu^2 = i\hbar$,

$\hbar \in \mathbb{R}$, $L = \frac{1}{2}\Delta$, $Y = eA$, $e \in \mathbb{R}$, ' V ' $= V + \frac{1}{2}|Y|^2$, $W = \frac{1}{2}\mathrm{div}Y$ and ' S_0 ' $= eS_0$.

Observe that in this case the $M(t,r)$ are L^2 - isometries and K^μ is self adjoint .

<u>Proof of (4.10)</u>

By general principles , see the proof of Lemma 6B of **Elworthy and Truman** [1] and (19) of **Elworthy** , **Truman and Watling** [1] , we have the continuity equation :

$$\frac{\partial}{\partial t}\phi(t,s,q) + \mathrm{div}\{\phi(t,s,.)\,[\nabla S_t(.) - Y(.)]\}(q) = 0$$

$$\phi(s,s,q) = 1$$

But $\alpha(t,s,q) = \exp\{\int_0^{t-s} (\mathrm{div}Y - \Delta S_{t-u})(\Pi\theta_u\Pi_t^{-1}q)du\}$

$$= \exp\{\int_0^{t-s} (\mathrm{div}Y - \Delta S_{s+r})(\Pi\theta_{-r}\theta_{t-s}\Pi_t^{-1}q)du\}$$

satisfies from (2.15) :

$$\frac{\partial}{\partial t}\alpha(t,s,q) = (\mathrm{div}Y - \Delta S_t)(q)\alpha(t,s,q) + \langle d\alpha(t,s,.)(q), Y(q) - \nabla S_t(q)\rangle$$

$$= \mathrm{div}\{\alpha(t,s,.)\,[Y(.) - \nabla S_t(.)]\}(q)$$

and clearly $\alpha(s,s,q) = 1$. Whence we have equality from which the Proposition follows .

$\square$

§5 Formulae for the Cauchy Problem Exhibiting Semi-Classical Asymptotics

(5.0) The Problem

We wish to know the asymptotic behaviour as $\mu \to 0$ of the classical solution $f^{\mu}(t,q) = \{P^{\mu}(t)f^{\mu}_{\bullet}\}(q)$ of the following Cauchy problem for the diffusion equation :

$$\frac{\partial}{\partial t} f^{\mu}(t,q) = \{K^{\mu}f^{\mu}_{t}\}(q)$$

$$f^{\mu}(0,q) = f^{\mu}_{\bullet}(q) = T_{\bullet}(q)\exp(-\frac{S_{\bullet}(q)}{\mu^2})$$

where $T_{\bullet}$ is a smooth scalar valued function on M .

(5.1) Lemma

Under the same assumptions as Theorem (4.4) but restricting ourselves to the Cauchy System only , we have :

$$\frac{\partial}{\partial r}\{Q^{\mu}(t,t-r)M(t-r,0)g\}(q) = \mu^2\{\,Q^{\mu}(t,t-r)M(t-r,0)L(t-r)g\}(q)\ ,$$

where for $s\in I$: $L(s) = M(0,s)LM(s,0)$.

Proof

$$\{M(t-r,0)g\}(q) = g(\pi\theta_{t-r}\pi^{-1}_{t-r})\exp\{\int_0^{t-r}(W-L_{\bullet}(S_u))(\pi\theta_{-u}\theta_{t-r}\pi^{-1}_{t-r}q)du\ \}$$

So by (2.15) we have :

$$\frac{\partial}{\partial r}M(t-r,0)g = -(W-L_{\bullet}S_{t-r})M(t-r,0)g - \langle d(M(t-r,0)g)\ ,\ Y-A(dS_{t-r})\rangle$$

Thus result follows from (4.2.2) and definition of $L(t-r)$. $\square$

(5.2) <u>Remark</u>

Again it should be pointed out that this proposition is true for any scalar second order differential operator $\mathbb{L}$, μ any complex number , P^{μ} any semigroup associated with the corresponding $\mathbb{K}^{\mu}$ in the situation of (4.02) for the Cauchy System .

Also observe that in the situation of (4.11) , $\mathbb{L}(t)$ is simply the transport of $\mathbb{L}$ via the time inhomogenous classical flow on M when considered as an operator on L^2 .

(5.3) <u>Theorem</u>

For T_o of compact support and with the assumptions of lemma (5.1) , we have for all $N \geq 0$ and $t \in I$:

$$f^{\mu}(t,q)=\exp\left(-\frac{S(t,q)}{\mu^2}\right)\{a_o(t,q)+a_1(t,q)\mu^2+\ldots+a_N(t,q)\mu^{2N}+R^{\mu}_{N+1}(t,q)\mu^{2(N+1)}\} ,$$

where :

$$a_o(t,q) = \{M(t,0)T_o\}(q) ,$$

and for $n \geq 1$:

$$a_n(t,q) = \int_0^t \ldots \int_0^{r_{n-1}} \{M(t,0)\mathbb{L}(t-r_n)\ldots\mathbb{L}(t-r_1)T_o\}(q)\, dr_n \ldots dr_1 ,$$

and $R^{\mu}_{n+1}(t,q)$ is bounded independently of μ since it is given for $n \geq 0$ by :

$$R^{\mu}_{n+1}(t,q) = \int_0^t \ldots \int_0^{r_n} \{Q^{\mu}(t,t-r_{n+1})M(t-r_{n+1},0)\mathbb{L}(t-r_{n+1})\ldots\mathbb{L}(t-r_1)T_o\}(q)dr_{n+1}\ldots dr_1 ,$$

$$= E\left\{\int_0^t \cdots \int_0^{r_n} \{M(t-r_{n+1},0)\cdots T_e\}(x^{t,\mu}(r_{n+1}))\exp\left\{\int_0^{r_{n+1}}(W+\mu^2 U-L_e S_{t-u})(x^{t,\mu}(u))du\right\}dr_{n+1}\cdots dr_1\right\}$$

where $x^{t,\mu}$ is as in (4.4) .

Proof

By (5.1) we observe that for h smooth of compact support and $0 \le r \le t$ we have :

$$Q^{\mu}(t,t-r)M(t-r,0)h = Q^{\mu}(t,t)M(t,0)h + \int_0^r \frac{\partial}{\partial u}\{Q^{\mu}(t,t-u)M(t-u,0)h\}du$$

$$= M(t,0)h + \mu^2\int_0^r \{Q^{\mu}(t,t-u)M(t-u,0)L(t-u)h\}du$$

So taking $h=T_e$, $r=t$, and $u=r_1$ we see the Theorem is true for $n=0$.

Then proceed by induction : taking $h=\{L(t-r_{n+1})\ldots L(t-r_1)T_e\}$ which is again smooth of compact support , $r=r_{n+1}$ and $u=r_{n+2}$ we see that : $R^{\mu}_{n+1}(t,q) = a_{n+1}(t,q) + \mu^2 R^{\mu}_{n+2}(t,q)$, and whence the result .

The probabalistic representation of the remainder follows from (4.4) , from which we get the boundedness independently of μ .

$\square$

(5.4) Remark

Doss has obtained an asymptotic expansion in the case $M=\mathbb{R}^d$ and there exists a smooth $X:\mathbb{R}^d \to L(\mathbb{R}^n,\mathbb{R}^d)$ such that $L = \frac{1}{2}L_X^2$ and $W=0$. See Doss [3] .

(5.5) Remark

It should be noted that the formula for $Q^{\mu}(t,0)$ in this theorem will be true for μ any complex number , L any second order differential operator (i.e. not necessarily semi-elliptic) , P^{μ} any semigroup (i.e. not necessarily preserving smooth functions) associated with the corresponding K^{μ} in the situation of (4.0.2) for the Cauchy System : but we would not have any control over Q^{μ} and consequently no control over the 'Remainder ' term R^{μ} , so we could not deduce that this gave an asymptotic expansion . However if we knew for example that Q^{μ} had norm bounded independently of μ when it is considered as an operator on some appropriate function space (c.f. above with working in L^2 for the Quantum Mechanics in **Elworthy and Truman** [1] , **Elworthy , Truman and Watling** [1]) we could indeed deduce that this was an asymptotic expansion in that function space . We are essentially working in L^{∞} here , but if we were working in L^2 in the Schrödinger Equation case i.e. the situation mentioned in (4.11) , then we could deduce the results of **Elworthy , Truman and Watling** [1] from this Hamiltonian viewpoint as the gauge invariant Laplacian is expanded to show it is of the desired form K^{μ} (see (4.9) , (4.10) and (4.11)) .

§6 A Further Look at Some Semi-Classical Semigroups

(6.1) With the assumptions of Theorem (4.4) we define the operators :

$\{B^{\mu,\lambda}(t,s)\}(q) = \varphi(t,\lambda)(q)^{-1}\{Q^{\mu}(t,s)\varphi(s,\lambda)g\}(q)$, for $\lambda,t,s \in I$, with $\lambda \le s \le t$,

on scalar valued functions g on M for which the right hand side is defined : which will certainly include smooth g of compact support .

(6.2) Lemma

Formally these operators form a time inhomogenous semigroup i.e. : $B^{\mu,\lambda}(t,s)B^{\mu,\lambda}(s,r) = B^{\mu,\lambda}(t,r)$, for $\lambda,t,r,s \in I$, with $\lambda \le r \le s \le t$,and moreover for smooth g of compact support :

(6.2.1) $\frac{\partial}{\partial t}\{B^{\mu,\lambda}(t,s)g\}(q) = \{J^{\lambda}(t)B^{\mu,\lambda}(t,s)g\}(q)$, for $\lambda,t,s \in I$, with $\lambda \le s \le t$,

(6.2.2) $\frac{\partial}{\partial r}\{B^{\mu,\lambda}(t,t-r)g\}(q) = \{B^{\mu,\lambda}(t,t-r)J^{\lambda}(t-r)g\}(q)$, for $\lambda,t,t-r \in I$, with $\lambda \le t-r \le t$,

where $J^{\lambda}(s)$, $s \in I$ is the time dependent smooth scalar second order semi-elliptic differential operator :

$$\mu^2 L_e + \{Y - A(dS_s) + \mu^2 A(d\log\varphi(s,\lambda))\} + \mu^2 \frac{L\varphi(s,\lambda)}{\varphi(s,\lambda)}$$

Proof

(6.2.3) Firstly observe that we have by (2.15) :

$$\frac{\partial}{\partial t}\varphi(t,\lambda)(q) = (W - L_e S_t)(q)\varphi(t,\lambda)(q)$$
$$+ \varphi(t,\lambda)(q)\langle d\log\varphi(t,\lambda)(q), Y(q) - A(dS_t)(q)\rangle$$

as $\varphi(t,\lambda)(q) = \exp\{\int_0^{t-\lambda} (W - L_e S_{s+\lambda})(\Pi\theta_{-s}\theta_{t-\lambda}\Pi_t^{-1}q)\,ds\}$.

(6.2.1) For any smooth h of compact support we have :

$$\frac{\partial}{\partial t}\varphi(t,\lambda)(q)^{-1}\{Q^{\mu}(t,s)h\}(q) = \{\frac{\partial}{\partial t}\varphi(t,\lambda)(q)^{-1} + \varphi(t,\lambda)(q)^{-1}\frac{\partial}{\partial t}\{Q^{\mu}(t,s)h\}(q)\}$$

$$= \varphi(t,\lambda)(q)^{-2}\{-\frac{\partial}{\partial t}\varphi(t,\lambda)(q) + \varphi(t,\lambda)(q)\{\mathbb{I}(t)Q^{\mu}(t,s)h\}(q)\}\text{ , by (4.2.1)}$$

(6.2.4) For any smooth k and l we have the commutator :

$$[\mathbb{I}(t),\exp(k)](l) = \{\mu^2A(dk) + \langle dk,Y-A(dS_t)\rangle + \mu^2\mathbb{L}_o(k) - \mu^2Q(dk)\}(\exp(k)l)$$

$$= \exp(k)\{\mu^2A(dk) + \langle dk,Y-A(dS_t)\rangle + \mu^2\mathbb{L}_o(k) + \mu^2Q(dk)\}(l)$$

(6.2.5) $\mu^2\mathbb{L}_o(\exp(k))\ \} = \mu^2\mathbb{L}_o(k) + \mu^2Q(dk)\exp(k)$

So (6.2.1) follows by taking : $h = \varphi(s,\lambda)g$, $k = -\log\varphi(t,\lambda)$, $l = Q^{\mu}(t,s)h$ and using (6.2.3) (6.2.4) and (6.2.5) .(6.2.2) We have :

$$\frac{\partial}{\partial r}\varphi(t,\lambda)(q)^{-1}Q^{\mu}(t,t-r)\varphi(t-r,\lambda)g$$

$$= \varphi(t,\lambda)(q)^{-1}Q^{\mu}(t,t-r)\{\frac{\partial}{\partial r}\varphi(t-r,\lambda) + \mathbb{I}(t-r)\varphi(t-r,\lambda)\}g$$

by (4.2.2) : so (6.2.2) follows by taking : $k = \log\varphi(t-r,\lambda)$, $l = g$ and using (6.2.3) (6.2.4) and (6.2.5) .Alternatively we could use the semigroup property to prove one from the other , but observe that (4.2.2) does not require Q^{μ} to preserve smooth functions .

□

(6.3) <u>Remark</u>

For $\mathbb{L}$ any scalar second order differential operator , μ any complex number , Q^{μ} arising from any P^{μ} associated with the corresponding K^μ in the situation of (4.0.2) , (6.2.2) is true , and given that this P^μ preserves smooth functions (6.2.1) is true .

(6.4) <u>Theorem</u>

With the assumptions of (6.1) and further assuming $\varphi(u,\lambda)^{-1}L\varphi(u,\lambda)$, is bounded above uniformly in (u,λ) over any compact subinterval of $I\times I$, which is certainly true for M compact , we have for smooth g of compact support and for $\lambda, t-r, t \in I$ with $\lambda \le t-r \le t$:

$$\{B^{\mu,\lambda}(t,t-r)g\}(q) =$$

$$E[g(x^{t,\mu,\lambda}(r))\exp\{\int_0^r \mu^2(\varphi(t-u,\lambda)^{-1}L\varphi(t-u,\lambda))(x^{t,\mu,\lambda}(u))du\}]$$

where $x^{t,\mu,\lambda}(u)$ is the solution of the following stochastic differential equation that we assume to be non-explosive , as will certainly be the case given some bounds or if M is compact : if L is elliptic or we have some other reason to make a natural choice of connection then we will take it to mean an Itô equation with $X_0 = X_0(\nabla)$ as in (1.8) and X as in (1.10) : if we can choose a smooth X then we will take it to mean a Stratonovich equation with $X_0(X)$ as in (1.13) :

$$dx^{t,\mu,\lambda}(u) = \mu X(x^{t,\mu,\lambda}(u))dB(u)$$

$$+ [\mu^2 X_0 + Y - A(dS_{t-u}) + \mu^2 A(d\log\varphi(t-u,\lambda))](x^{t,\mu,\lambda}(u))du$$

$x^{t,\mu,\lambda}(0) = q$, where B(u) is Brownian Motion on $\mathbb{R}^n$.

(6.5) Remarks

(6.5.1) This enables us to extend the domain of the $B^{\mu,\lambda}(t,s)$ to say bounded and measurable functions g as the right hand side makes sense for such functions , They then form a semigroup on this function space .

(6.5.2) When L is Elliptic we could express $x^{t,\mu,\lambda}(u)$ as the projection of the solution of a canonical Stratonovich equation on O(M) as indicated in (1.14) and then the case of this Theorem for the K^{μ} Cauchy System with : $\lambda = 0$, $r = t$, $L_a = \frac{1}{2}\Delta$, $Y = 0$ and $W = 0$,will be the 'Elementary Formula B' of **Elworthy and Truman** [2] : the case of the theorem with r=t could indeed have been obtained by use of Feynman-Kac-Girsanov transformations as in this reference however the semi-classical semigroup approach makes the iteration process in the next chapter easier to see and clarifies the similarities with the semi-classical analysis of the Schrödinger equation as in **Elworthy and Truman** [1] and **Elworthy , Truman and Watling** [1] . See also (4.9) -(4.11) .

Proof of (6.4)

Define $h : [t-r,t]\times M\times\mathbb{R}\to\mathbb{R}$ by : $h(u,q,v)=v\{B^{\mu,\lambda}(u,t-r)g\}(q)$, then :

(6.4.1) $\frac{\partial}{\partial u}h(u,q,v) = \{J^{\lambda}(t)h(u,v)\}(q)$, by (6.2.1) .

Consider the Process $y^{t,\mu,\lambda}(u) = (\tau^t(u)\ ,\ x^{t,\mu,\lambda}(u)\ ,\ v^{t,\mu,\lambda}(u))$ on the domain of h given by the stochastic differential equation :

$$dx^{t,\mu,\lambda}(u) = \mu X(x^{t,\mu,\lambda}(u))dB(u)$$

$$+ [\mu^2 X_0 + Y - A(dS(\tau^t(u))) + \mu^2 A(d\log\varphi(\tau^t(u),\lambda))](x^{t,\mu,\lambda}(u))du$$

$$d\tau^t(u) = -du$$

$dv^{t,\mu,\lambda}(u) = [\mu^2(\varphi(t,\lambda)^{-1}L\varphi(t,\lambda))(x^{t,\mu,\lambda}(u))]$ [redacted] $v^{t,\mu,\lambda}(u)du$

with : $x^{t,\mu,\lambda}(0) = q\ ,\ \tau^t(0) = t\ ,\ v^{t,\mu,\lambda}(0) = 1$.

So $\tau^t(u) = t-u$ and $v^{t,\mu,\lambda}(u) = \exp\{\int_0^u \mu^2(\varphi(t-s,\lambda)^{-1}L\varphi(t-s,\lambda))(x^{t,\mu,\lambda}(s))ds\}$

and the result follows by applying Ito's Formula to $h(y^{t,\mu,\lambda}(u))$ using (6.4.1) and taking expectations as in the proof of (4.4).

$\square$

(6.6) Remark

This theorem certainly uses the facts that μ is real , L is semi-elliptic and that P^μ preserves smooth functions .

(6.7) Remark

If : $L = \frac{1}{2}\Delta + b + c$, $Y = 0$ and $W = V = 0$, where b is a vector field on M and c is a real valued function , then for the Kernel System with $\Gamma_e = T^*M_y$ we have from (4.10):

$$\varphi(r,\lambda)(q) = \sqrt{\phi(r,\lambda)(q)}\ \exp\{\int_0^{r-\lambda} -(bS_{r-u})(\Pi\theta_u\Pi_r^{-1}q)du\ \}$$

$$= \sqrt{|\det T_q(\Pi\theta_{r-\lambda}\Pi_r^{-1})|}\exp\{\int_0^{r-\lambda}\langle b(\Pi\theta_u\Pi_r^{-1}q),-dS_{r-u}(\Pi\theta_u\Pi_r^{-1}q)\rangle du\}$$

$$=\{\sqrt{(\lambda r^{-1})^d}\}\theta_y^{-1}(\lambda r^{-1}\exp_y^{-1}q)\theta_y(\exp_y^{-1}q)\exp\{\int_0^{r-\lambda}\langle b(\Pi\theta_u\Pi_r^{-1}q),\theta_u\Pi_r^{-1}q)\rangle du\}$$

$$=\{\sqrt{(\lambda r^{-1})^d}\}\theta_y^{-1}(\lambda r^{-1}x)\theta_y(x)\exp\{\int_0^{r-\lambda}\langle b(\alpha(u)),\alpha'(u))\rangle du\},$$

where x is q expressed in the global normal cooordinates assumed to exist as a consequence of the Kernel No Caustics Assumption of (2.11.2) , $\theta_y: TM_y \to (0,\infty)$ is the square root of the inverse of Ruse's Invariant which is the Jacobian determinant of the exponential map $\exp_y: TM_y \to M$ see **Elworthy and Truman** [1] , and $\alpha(u)$ is the unique geodesic from q to y parameterised to take time r .

Also observe that :

$$S_r(q) = \frac{d(q,y)^2}{2r}, \text{ where } d \text{ denotes the Riemannian distance .}$$

We then make the following observations :

(6.7.1) $$\lim_{\lambda\to 0}\frac{\phi(r,\lambda)(q)}{(\sqrt{\lambda})^d} = \frac{1}{(\sqrt{r})^d}\theta_y(q)\exp\{\int_0^r\langle b(\alpha(u)),\alpha'(u))\rangle du\},$$

$$= \frac{1}{(\sqrt{r})^d}\theta_y(q)\exp\{\int_0^1\langle b(\gamma(u)),\gamma'(u))\rangle du\},$$

Where γ is the unique geodesic from q to y parameterised to take time 1 .

Also notice that : $\frac{1}{(\sqrt{r})^d}\Theta_\gamma(q) = \sqrt{|\det T_q(\theta_r \Pi_r^{-1})|}$.

Let $B_\gamma(q) = \exp\{\int_0^1 \langle b(\gamma(u)),\gamma'(u)\rangle du\}$, and $C_\gamma(q) = B_\gamma(q)\Theta_\gamma(q)$ then we have :

(6.7.2) $\lim_{\lambda\to 0} \nabla\log\varphi(r,\lambda)(q) = \nabla\log\Theta_\gamma(q) + \nabla\log B_\gamma(q) = \nabla\log C_\gamma(q)$, and

(6.7.3) $\lim_{\lambda\to 0} \frac{L\varphi(r,\lambda)(q)}{\varphi(r,\lambda)(q)} = \frac{LC_\gamma(q)}{C_\gamma(q)}$

Thus $\lim_{\lambda\to 0}\{B^{\mu,\lambda}(t,t-r)g\}(q)$ looks like a semigroup $B^\mu(t,t-r)$ acting on g ,

where $\{B^\mu(t,s)g\}(q) = \frac{(\sqrt{t})^d}{(\sqrt{s})^d}\frac{\{Q^\mu(t,s)C_\gamma\}(q)}{C_\gamma(q)}$.

Moreover it looks like we have the following probabalistic representation from (6.4) :

$$\{B^\mu(t,t-r)g\}(q) = E[g(x^{t,\mu}(r))\exp\{\int_0^r \mu^2 \frac{LC_\gamma}{C_\gamma}(x^{t,\mu}(u))du\}],$$

where $x^{t,\mu}(r)$ is the solution of the following Itô Equation with respect to the Levi-Civita connection :

$$dx^{t,\mu}(u) = \mu X(x^{t,\mu}(u))dB(u) + [\mu^2 b - \nabla S_{t-u} + \mu^2\nabla\log C_\gamma](x^{t,\mu}(u))du ,$$

$$x^{t,\mu}(0) = q .$$

As we shall see in §7 it is easy to observe that :

$$\lim_{s\to 0}\{B^\mu(t,s)g\}(q) = \exp(\frac{S(t,q)}{\mu^2})C_\gamma(q)^{-1}\{\sqrt{(2\pi t\mu^2)^d}\}g(y)p^\mu(t,q,y) .$$

Moreover we will see that the process $x^{t,\mu}(r)$ is a 'Bridge' process between q and y which certainly looks like a Doob h-Transform of the diffusion process associated with L_{*} . So by taking g such that g(y)=1 we are lead to a formula for the heat kernel $p^{\mu}(t,q,y)$.

This motivates our approach in §7 to the small time behaviour of the Heat Kernel of an Elliptic Operator .

(6.8) Remark

The approach of **Elworthy and Truman** [2] to the situation Of (6.7) where furthermore b=0 consisted of studying $\{B^{\mu,\lambda}(t+\lambda,\lambda)g\}(q)$ as $\lambda \to 0$ while we will sidestep two of these λ limits by starting by defining the semigroup $B^{\mu}(t,s)$ which has a natural probabalistic interpretation and finally taking the other limit i.e. $s \to 0$; this also has the advantage that higher order formulae for the heat kernel can also be obtained .

§7 Formulae for the Heat Kernel of an Elliptic Operator Exhibiting Small Time Asymptotics

(7.0) The Problem

Given a smooth scalar second order elliptic differential operator L on a smooth connected d – dimensional manifold M we have a natural choice of smooth Riemannian Structure as described in (1.6).

We wish to study the small time behaviour of the fundamental solution (Heat Kernel) $p(t,x,y)$ of the Heat Equation :

$$\frac{\partial f}{\partial t}(t,x) = Lf_t(x) ,$$

with respect to the natural Riemannian Measure .

(7.1) The No-Caustics Assumption

We assume that y is a pole of the natural Riemannian manifold i.e. the exponential map based at y is a diffeomorphism , so there is a unique geodesic parameterised to take unit time between y and any point of the manifold .

(7.2) Notation

(7.2.1) As described in (1.7) , (1.8) and (1.9) we may write :

$$L = \tfrac{1}{2}\Delta + b + c ,$$

where Δ is the Laplace-Beltrami operator for the natural Riemannian Structure , b is a smooth vector field on M , and c is a real valued function on M .

With the assumption of (7.1) we may define the following functions on M motivated by the discussion in (6.7) :

(7.2.2) $\Theta_y(x)$ = the square root of the Jacobian determinant with respect to the natural Riemannian structure of the inverse of the exponential map based at y , at the point x ,

(7.2.3) $B_y(x) = \exp\{\int_0^1 \langle\gamma'(u),b(\gamma(u))\rangle du\}$,

where γ is the unique geodesic from x to y parameterised to take unit time and γ' is its velocity , (the integrand is the work done by b in moving along the geodesic γ) ,

(7.2.4) $C_y(x) = \Theta_y(x)\, B_y(x)$,

(7.2.5) $D_y(x) = \frac{1}{2}d(x,y)^2$,

where d(x,y) is the natural Riemannian distance between x and y , ($D_y(x)$ is the energy of the geodesic γ) .

Finally we may define the following functions on $\mathbb{R}^+ \times M$:

(7.2.6) $r_y(t,x) = \frac{1}{\sqrt{(2\pi t)^d}}\Theta_y(x)\, \exp\{-\frac{1}{t}D_y(x)\}$,

(7.2.7) $q_y(t,x) = B_y(x) r_y(t,x)$.

(7.3) Remark

We need the important fact from Elworthy [1] (Chapter IX §12 Example 12D) that if f(x) is a real valued function on M which depends only on r = d(x,y) (i.e. it is invariant under rotations about y) then :

$$(7.3.1)\ \Delta f(x) = \frac{d^2 f}{dr^2}(r) + \left\{ \frac{d-1}{r} - 2\frac{\partial}{\partial r}\log\Theta_y(x) \right\} \frac{df}{dr}(r).$$

(7.4) Lemma

$$\frac{\partial}{\partial t} r_y(t,x) = \frac{1}{2}\Delta r_y(t,x) - \frac{\Delta\Theta_y(x)}{2\Theta_y(x)} r_y(t,x),$$

Proof

Using the fact that $\Delta\exp(f) = (\Delta f + \|\nabla f\|^2)\exp(f)$, for real valued functions f on M, we see that :

$$\Delta r_y(t,x) = \{ \Delta(\log\Theta_y - \tfrac{1}{t}D_y)(x) + |\nabla\log\Theta_y(x) - \tfrac{1}{t}\nabla D_y(x)|^2 \} r_y(t,x)$$

$$= \{\Delta(\log\Theta_y)(x) - \tfrac{1}{t}\Delta D_y(x) - \tfrac{2}{t}\langle\nabla\log\Theta_y(x),\nabla D_y(x)\rangle + \|\nabla\log\Theta_y(x)\|^2$$

$$+\frac{1}{t^2}\|\nabla D_y(x)\|^2 \} r_y(t,x)$$

So from (7.3.1) applied to D_y and using the facts that :

$$\Delta f = (\Delta(\log f) + \|\nabla\log f\|^2)f,$$

for real valued functions f on M, and :

$$\|\nabla Dy(x)\|^2 = 2D_y(x),$$

we deduce that :

$$\frac{1}{2}\Delta r_y(t,x) = \{ \frac{\Delta\Theta_y(x)}{2\Theta_y(x)} - \frac{d}{2t} + \frac{1}{t^2} D_y(x) \} r_y(t,x)$$

$$= \frac{\Delta\Theta_y(x)}{2\Theta_y(x)} r_y(t,x) + \frac{\partial}{\partial t} r_y(t,x)$$

□

(7.5) <u>Proposition</u>

If $p_y(t,x,z)$ is the fundamental solution of the heat equation :

$$\frac{\partial f}{\partial t}(t,x) = Lf_t(x) - \frac{LC_y(x)}{C_y(x)} f_t(x) ,$$

with respect to the natural Riemannian measure .

Then $p_y(t,x,y) = q_y(t,x)$.

<u>Proof</u>

As in **Elworthy and Truman** [1] , **Elworthy** [1] (Chapter IX §12B) , we see that $q_y(t,x)$ (considered as a distribution with respect to the natural Riemannian measure) tends to the delta function at y as t tends to 0 , by a simple change of variable argument .

By (7.4) and the fact that $\Delta(fg) = f\Delta g + g\Delta f + 2\langle \nabla f, \nabla g \rangle$, for real valued functions f and g :

$$\frac{\partial}{\partial t} q_y(t,x) = B_y(x)\left\{\frac{1}{2}\Delta r_y(t,x) - \frac{\Delta\Theta_y(x)}{2\Theta_y(x)} r_y(t,x)\right\},$$

$$= \frac{1}{2}\Delta q_y(t,x) + \left\{\frac{1}{t}\langle \nabla \log B_y(x), \nabla D_y(x)\rangle - \frac{\Delta C_y(x)}{2C_y(x)}\right\} q_y(t,x) ,$$

$$= Lq_y(t,x) + \left\{\frac{1}{t}\langle b(x) + \nabla \log B_y(x), \nabla D_y(x)\rangle - \frac{LC_y(x)}{C_y(x)}\right\} q_y(t,x) ,$$

(7.5.1) Observe that if b is a gradient then $b + \nabla \log B_y = 0$, so in this case we have the result .

In general we will prove that :

(7.5.2) $\langle b(x) + \nabla \log B_y(x) , \nabla D_y(x) \rangle = 0$.

i.e. $b + \nabla \log B_y$ only rotates about y .

Firstly note that we have $\nabla D_y(x) = \gamma'(0)$, where γ is the unique geodesic from x to y parameterised to take unit time , so :

$$\langle \nabla \log B_y(x) , \nabla D_y(x) \rangle = \frac{d}{dr} \log B_y(\gamma(r)) \Big|_{r=0}$$

But :

$$\log B_y(\gamma(r)) = \int_0^1 \langle \alpha'(u), b(\alpha(u)) \rangle du ,$$

where α is the unique geodesic from $\gamma(r)$ to y parameterised to take unit time ,

$$= \int_r^1 \langle \gamma'(s), b(\gamma(s)) \rangle ds \quad \text{, where } \gamma \text{ is as above ,}$$

so : $\frac{d}{dr} \log B_y(\gamma(r)) \Big|_{r=0} = -\langle \gamma'(0) , b(\gamma(0)) \rangle = -\langle \nabla D_y(x) , b(x) \rangle$,

whence the result .

□

(7.6) Let $P(t)$ be the semigroup associated with $p(t,x,y)$. Define the operators $Q_y(t,s)$ by :

(7.6.1) $\{Q_y(t,s)f\}(x) = q_y(t,x)^{-1} \{ P(t-s) (q_y(s, .) f(.)) \}(x)$,

for $t \geq s > 0$, on smooth functions of compact support .

(7.7) Remark

(7.7.1) Formally these operators form a two parameter semigroup i.e. :

$$Q_y(t,s)\, Q_y(s,r) = Q_y(t,r)\,, \text{ for } t \geq s \geq r > 0\,.$$

(7.7.2) This is like a Doob h-transform of the semigroup P(t) but with respect to a function q_y on space-time that is only ' approximately harmonic ' for the operator : $\frac{\partial}{\partial t} - L$, with 'error' given by (7.5) .

(7.8) Lemma

For f smooth of compact support we have :

(7.8.1) $\frac{\partial}{\partial s}\{Q_y(t,t-s)f\}(x) = \{Q_y(t,t-s)(I_y(t-s)f)\}(x)$, for $t > s \geq 0$, and

(7.8.2) $\frac{\partial}{\partial t}\{Q_y(t,s)f\}(x) = \{I_y(t)(Q_y(t,s)f)\}(x)$, for $t \geq s > 0$,

where $\{I_y(t)f\}(z) = \{L_o f\}(z) + \langle \nabla \log q_y(t,z)\,,\, \nabla f(z)\rangle + \frac{LC_y(z)}{C_y(z)}\, f(z)$,

(7.8.3) $$= \frac{L(\,C_y\, f)(z)}{C_y(z)} - \frac{1}{t}\langle \nabla D_y(z)\,,\, \nabla f(z)\rangle$$

(7.8.4) $$\begin{aligned} &= \frac{1}{2}\Delta f(z) + \langle \nabla \log \Theta_y(z) + (b + \nabla \log B_y)(z) - \frac{1}{t}\nabla D_y(z)\,,\, \nabla f(z)\rangle \\ &\quad + \{\, \frac{\Delta \Theta_y(z)}{2\Theta_y(z)} + \frac{1}{2}\Delta \log B_y(z) + \langle \nabla \log \Theta_y(z)\,,\, (b + \nabla \log B_y)(z)\,\rangle \\ &\quad + \frac{1}{2}\|\nabla \log B_y(z)\|^2 + \langle b(z)\,,\, \nabla \log B_y(z)\,\rangle + c(z)\,\}f(z) \end{aligned}$$

In particular when b is a gradient we have :

$$(7.8.5)\quad \{\mathbb{I}_y(t)f\}(z) = \tfrac{1}{2}\Delta f(z) + \langle \nabla \log r_y(t,z), \nabla f(z)\rangle$$

$$+ \left\{ \frac{\Delta\theta_y(z)}{2\theta_y(z)} - \frac{1}{2}\operatorname{div} b(z) - \frac{1}{2}|b(z)|^2 + c(z) \right\} f(z)$$

<u>Proof</u>

By (7.5) and definition of P we have :

$$\frac{\partial}{\partial s}\{Q_y(t,t-s)f\}(x)$$

$$= Q_y(t,t-s)\left\{ \frac{\mathbb{L}(q_y(t-s,.)f(.))}{q_y(t-s,.)} - \frac{\mathbb{L}(q_y(t-s,.))}{q_y(t-s,.)} f(.) + \frac{\mathbb{L}C_y(.)}{C_y(.)} f(.) \right\}(x)$$

whence (7.8.1) follows from the fact that :

$$\Delta(fg) = f\Delta g + g\Delta f + 2\langle \nabla f, \nabla g\rangle ,$$

for real valued functions f and g .

Similarly :

$$\frac{\partial}{\partial t}\{Q_y(t,s)f\}(x) = \frac{\mathbb{L}(q_y(t,.)(Q_y(t,s)f)(.))(x)}{q_y(t,x)}$$

$$- \frac{\mathbb{L}q_y(t,x)}{q_y(t,x)}\{Q_y(t,s)f\}(x) + \frac{\mathbb{L}C_y(x)}{C_y(x)}\{Q_y(t,s)f\}(x)$$

whence (7.8.2) follows as above .

Finally (7.8.3) follows from the same identity , (7.8.4) from the definitions of $\mathbb{L}$ and C_y , and (7.8.5) from (7.5.1) .

□

(7.9) Definition

The q_y-transformed L_* diffusion $x^t(u)$ starting from x is the time dependent diffusion with generator for $t>u\geq 0$:

$$L_*(z) + \nabla \log q_y(t-u,z) = \tfrac{1}{2}\Delta(z) + b(z) + \nabla \log q_y(t-u,z) ,$$

which may be represented as a strong solution of a stochastic differential equation . By (1.12.1) we can find a smooth $X:M\to L(\mathbb{R}^n,TM)$ such that $A=XX^*$ is the symbol of L defined in (1.2) . Then $x^t(u)$ is the solution of the following Itô differential equation with respect to the Levi-Civita connection :

$$dx^t(u) = X(x^t(u))\, dB(u) + \{b(x^t(u)) + \nabla \log q_y(t-u,x^t(u))\}\, du ,$$

$x^t(o) = x$,where B(u) is n dimensional Brownian Motion .

(7.10) Remark

(7.10.1) If b is a gradient vector field then from (7.8.5) we see that $x^t(u)$ is actually Brownian motion on M transformed with respect to r_y , i.e it is the Brownian Riemannian Bridge Process of **Elworthy and Truman** [1] and **Elworthy** [1] (Chapter IX §12D) , which might also be called the semi-classical bridge process for this situation . So $x^t(u)$ tends to y almost surely as u increases to t and consequently the process does not explode .

(7.10.2) For more general b we get a different process , but as we will see in (7.11) , (7.5.2) means that the same argument as in **Elworthy** [1] (Chapter IX §12D) will show that it is a bridge process which is radially the same as the Euclidean Brownian Bridge in $\mathbb{R}^d$: so in particular $x^t(u)$ tends to y almost surely as u increases to t and consequently this process does not explode either .

(7.11) Lemma

The q_y - transformed L_a diffusion $x^t(u)$ is a bridge process , i.e. $x^t(u)$ tends to y almost surely as u increases to t , whose radial component has the same law as the Euclidean Brownian Bridge in $TM_y \cong \mathbb{R}^d$ between $\exp_y^{-1}x$ and 0 in time t .

Proof

Consider the function $R_y : M \to \mathbb{R}$ defined by $R_y(x) = d(x,y)$. Then we see that R_y is C^2 on $M-\{y\}$ while for $d\geq 2$ and $x\neq y$ we have that almost surely $x^t(u)$ avoids y for $0\leq u<t$. So we may apply Itô's formula for $0\leq u<t$ to deduce that :

$$R_y(x^t(u)) = R_y(x) + \int_0^u \langle \nabla R_y(x^t(s)), X(x^t(s))dB(s)\rangle$$

$$+ \int_0^u \langle \nabla R_y(x^t(s)), b(x^t(s)) + \nabla \log q_y(t-s, x^t(s))\rangle ds + \int_0^u \frac{1}{2}\Delta R_y(xt(s))ds$$

From (7.3.1) applied to R_y we see that :

$$\Delta R_y(z) = \frac{d-1}{R_y(z)} - 2\frac{\partial}{\partial r}\log\theta_y(z) .$$

From (7.5.1) and the observation that $\nabla D_y(z) = R_y(z)\nabla R_y(z)$ we see that :

$$\langle \nabla R_y(z) \, , \, b(z) + \nabla \log B_y(z) \rangle = 0 \, .$$

As $\|\nabla R_y(z)\|^2 = 1$ we see that :

$$\langle \nabla R_y(z) \, , \, \nabla D_y(z) \rangle = R_y(z) \, .$$

If we define :

$$W^t(u) = \int_0^u \langle \nabla R_y(x^t(s)) \, , \, X(x^t(s)) dB(s) \rangle \, ,$$

then we see that it is a 1 dimensional Brownian Motion from **Elworthy** [1] (Chapter V Corollary 5C) since if we define $H : M \to L(\mathbb{R}^n, \mathbb{R})$ by $H(z)(v) = \langle \nabla R_y(z) \, , \, X(z)v \rangle$ then $H^*(z) = X^*(z)(dR_y(z))$ so we have $HH^* = \|\nabla R_y(z)\|^2 = 1$.

Thus denoting $R_y(x^t(s))$ by $r^t(s)$ we see that $r^t(s)$ satisfies :

$$r^t(u) = r^t(0) + W(u) + \frac{1}{2}(d-1)\int_0^u \frac{ds}{r^t(s)} - \int_0^u \frac{r^t(s)}{t-s} \, ds \, .$$

Consequently it is just the radial component of the Euclidean Bridge in the statement of the Lemma . It then follows that $x^t(u)$ is a bridge process .

□

(7.12) Proposition

Assume $\dfrac{LC_y}{C_y}$ is bounded above on M , then for f smooth of compact support and $t>s\geq 0$ we have :

$$\{Q_y(t,t-s)f\}(x) = E_x\{\ f(x^t(s)) \exp\{\ \int_0^s \frac{LC_y(x^t(u))}{C_y(x^t(u))}\,du\ \}\ \}$$

where $x^t(u)$ is the q_y-transformed L_o diffusion starting from x .

(7.13) Remark

This enables us to extend the domain of the $Q_y(t,s)$ to say bounded measurable functions f as the right hand side of the above equality make sense for such functions . They then form a semigroup on this function space .

Proof (Of (7.12))

Define $h:[t-s,t]\times M\times\mathbb{R}\to\mathbb{R}$ by $h(r,x,v) = v\{Q_y(r,t-s)f\}(x)$. Notice this is smooth . Then :

$$\frac{\partial h}{\partial r}(r,x,v) = \{I_y(r)h(r,.,v)\}(x)\ ,\ \text{by (7.8.2)}\ .$$

Consider the process $y^t(r) = (\tau^t(r),x^t(r),v^t(r))$ on the domain of h given by :

$$d\tau^t(r) = -dr$$

$$dx^t(r) = X(x^t(r))dB(r) + \{\ b(x^t(r)) + \nabla\log q_y(\tau^t(r),x^t(r))\ \}\ dr$$

$$dv^t(r) = \frac{LC_y(x^t(r))v^t(r)}{C_y(x^t(r))}\,dr$$

with $x^t(0) = x$, $\tau^t(0) = t$, and $v^t(0) = 1$.

So :

$\tau^t(r) = t-r$, and

$$v^t(r) = \exp\{ \int_0^r \frac{LC_y(x^t(u))}{C_y(x^t(u))}\,du \} .$$

So the result follows by applying Itô's formula to $h(y^t(s))$ observing the cancellation that occurs to get :

$$v^t(s)\, f(x^t(s)) = \{Q_y(t,t-s)f\}(x) + M(s) ,$$

where $M(s)$ is a martingale , with $M(0) = 0$.

Then take expectations , observing that the martingale part must be bounded as the other non-constant term is by assumption , to deduce the result .

□

(7.14) Theorem

Recalling the definitions in (7.2) we assume $\frac{LC_y}{C_y}$ is bounded above on M ,

then for $t>0$:

$$p(t,x,y) = q_y(t,x)\, E_x\{\exp\int_0^t \frac{LC_y(x^t(u))}{C_y(x^t(u))}\,du\} ,$$

where $x^t(u)$ is the q_y-transformed L_0-diffusion starting from x .

<u>Proof</u>

Recalling (7.5) , (7.6.1) and (7.11) simply let s tend to t in (7.12) and use dominated convergence for f a smooth function of compact support taking the constant value one in a neighbourhood of the geodesic segment between x and y .

$\square$

(7.15) <u>Remark</u>

This is just the elementary formula of **Elworthy and Truman** [1] and **Elworthy** [1] (Chapter IX §12 Theorem 12D) in the case that $b=0$.

(7.16) <u>Definition</u>

For $0 \le r \le s$ let $F(s,r)$ be the operator : $\{F(s,r)f\}(z) = f(\gamma(s-r))$, where γ is the unique geodesic from z to y parameterised to take time s . These form a two parameter semigroup on , for example , bounded measurable functions .

(7.17) <u>Lemma</u>

Assume $\dfrac{LC_y}{C_y}$ is bounded above on M , then for f smooth and of compact support we have :

$$\frac{\partial}{\partial s}\{Q_y(t,t-s)F(t-s,t-r)f\}(x) = \{Q_y(t,t-s)(L_{C_y}F(t-s,t-r)f)\}(x) ,$$

for $t>r\geq s\geq 0$,where L_{C_y} is the operator defined by :

$$\{L_{C_y}g\}(z) = \frac{L(C_y(.)g(.))(z)}{C_y(z)} .$$

Proof

Follows from (7.8.3) and definition of $F(t-s,t-r)$.

□

(7.18) Proposition

Assume $\frac{LC_y}{C_y}$ is bounded above on M , then for f a smooth function of compact support taking the constant value one in a neighbourhood of the geodesic segment between x and y , we have for any $N\geq 0$ and $0\leq s<t$:

$$\{Q_y(t,t-s)f\}(x) = 1 + a_1(s,x,y) + \dots + a_N(s,x,y) + F_{N+1}(s,x,y) ,$$

where for $1\leq n\leq N$:

$$a_n(s,x,y) = \int_0^s \dots \int_0^{s_{n-1}} \{F(t,t-s_n)L_{C_y}\dots F(t-s_2,t-s_1)\frac{LC_y(.)}{C_y(.)}\}(x)\, ds_n \dots ds_1 ,$$

and for $1\leq n\leq N+1$:

$F_n(s,x,y) =$

$$E_x\{ \int_0^s \dots \int_0^{s_{n-1}} \{L_{C_y}\dots L_{C_y}F(t-s_1,t-s)f\}(x^t(s_n)) \exp(\int_0^{s_n} \frac{LC_y(x^t(u))}{C_y(x^t(u))}\, du) ds_n \dots ds_1\} ,$$

where $x^t(u)$ is the q_y transformed L_* diffusion .

Proof

By (7.17) for any smooth h of compact support , and any $0 \le r \le s$:

$$\{Q_y(t,t-r)h\}(x) = \{Q_y(t,t-r)F(t-r,t-r)h\}(x)$$

$$= \{Q_y(t,t)F(t,t-r)h\}(x) + \int_0^r \{Q_y(t,t-v)L_{C_y}F(t-v,t-r)h\}(x)dv$$

$$= \{F(t,t-r)h\}(x) + \int_0^r E_x\{ L_{C_y}[F(t-v,t-r)h](x(v)) \exp\{ \int_0^v \frac{LC_y(x^t(u))}{C_y(x^t(u))} du\} \} dv ,$$

by (7.11) .

So taking $h=f$, $r=s$ and $v=s_1$ we see the theorem is true for $N=0$.

Then we proceed by induction : taking ,

$$h = L_{C_y}F(t-s_n,t-s_{n-1})L_{C_y}...L_{C_y}F(t-s_1,t-s)f ,$$

which again is smooth of compact support , $r=s_n$ and $v=s_{n+1}$ we see that :

$$F_n(s,x,y) = a_n(s,x,y) + F_{n+1}(s,x,y)$$

and whence the result .

$\square$

(7.19) Definition

For $0 \le r \le s \le 1$ let $G(s,r)$ is the operator defined as : $(G(s,r)f)(z) = f(\alpha(s-r))$, where α is the unique geodesic from z to y parameterised to take time (1-r) . These form a two parameter semigroup on , for example , bounded measurable functions .

(7.20) Theorem

Recalling the definitions in (7.2) we assume $\frac{LC_y(z)}{C_y(z)}$ is bounded then we have for $N \geq 0$, provided that

$$\{ L_{C_y} G(r_{n-1}, r_n) \dots L_{C_y} G(r_1, r_2) \frac{LC_y(\,.\,)}{C_y(\,.\,)} \}(z) \text{, for } 0 \leq r_n \leq r_{n-1} \leq \dots \leq r_1 \leq 1$$

is bounded for $2 \leq n \leq N+1$:

$$p(t,x,y) = q_y(t,x)\{1 + a_1(x,y)t + a_2(x,y)t^2 + \dots + a_N(x,y)t^N + R_{N+1}(t,x,y)t^{N+1}\}$$

$$\text{where } a_1(x,y) = \int_0^1 \{ G(r_1, 0) \frac{LC_y(\,.\,)}{C_y(\,.\,)} \}(x)\, dr_1$$

and for $n \geq 2$:

$$a_n(x,y) = \int_0^1 \dots \int_0^{r_{n-1}} \{ G(r_n, 0) L_{C_y} G(r_{n-1}, r_n) L_{C_y} \dots G(r_1, r_2) \frac{LC_y(\,.\,)}{C_y(\,.\,)} \}(x)\, dr_n \dots dr_1 \text{ ,}$$

$$\text{and where } R_1(t,x,y) = E_x\{ \int_0^1 \frac{LC_y(x^t(tr_1))}{C_y(x^t(tr_1))} \exp\{\int_0^{tr_1} \frac{LC_y(x^t(u))}{C_y(x^t(u))}\, du\}\, dr_1\}$$

and for $n \geq 2$:

$R_n(t,x,y) =$

$$E_x\{\int_0^1 \dots \int_0^{r_{n-1}} \{L_{C_y} G(r_{n-1}, r_n) \dots \frac{LC_y(.)}{C_y(.)} \}(x^t(tr_n)) \exp\{\int_0^{tr_n} \frac{LC_y(x^t(u))}{C_y(x^t(u))}\, du\} dr_n \dots dr_1\}$$

where $x^t(u)$ is q_y-transformed L_e diffusion .

Observe that $R_n(t,x,y)t^{n+1}$ is $o(t^n)$ as t tends to 0 , so the above formula gives the asymptotic expansion of $p(t,x,y)$ as t tends to 0 .

Proof

Recalling (7.5) and (7.6.1) simply let s tend to t in (7.18) using dominated convergence for remainder term and finally change variables .

$\square$

(7.21) Example (Minakshishundaram-Pleijel Expansion)

We calculate the first term from Theorem (7.20) of $p(t,y,y)$ in the case c = 0 :

$$a_1(y,y) = \int_0^1 \{G(r,0)\,\underline{LC_y(\,.\,)}\}(y)\,dr \text{ [redacted] } = \underline{LC_y(y)},\ \text{as } G(r,0) = \text{Identity}.$$
$$\qquad\qquad\qquad\quad C_y(\,.\,) \qquad\qquad\qquad\qquad\quad C_y(y)$$

$$= \tfrac{1}{2}\Delta\theta y(y) - \tfrac{1}{2}\mathrm{div}\,b(y) - \tfrac{1}{2}\|b(y)\|^2,\ \text{as } (b + \nabla\log B_y)(y) = 0 \text{ and } \theta_y(y) = 1$$

$$= \tfrac{1}{12}S(y) - \tfrac{1}{2}\mathrm{div}\,b(y) - \tfrac{1}{2}\|b(y)\|^2,$$

where S is the Scalar curvature , see Besse [1] .

(7.22) Example (Hyperbolic n-space)

For hyperbolic n-space with constant sectional curvatures $-R^{-2}$ we have :

$$\theta_y(x) = \sqrt{\left(\frac{r/R}{\sinh(r/R)}\right)^{n-1}} = \sqrt{\{r/\psi(r)\}^{n-1}},$$

for $r = d(x,y)$ and $\psi(r) = R\sinh(r/R)$ .So by (7.3.1) applied to θ_y we see that :

$$\frac{\Delta\theta_y(x)}{2\theta_y(x)} = -\frac{(n-1)\psi''(r)}{4\ \psi(r)} + \frac{(n-1)(n-3)}{8}\left\{\frac{1}{r^2} - \frac{\psi'(r)^2}{\psi(r)^2}\right\}$$

$$= -\frac{(n-1)}{4R^2} + \frac{(n-1)(n-3)}{8}\left\{\frac{1}{r^2} - \frac{1}{\{R\tanh(r/R)\}^2}\right\}$$

$$= -\frac{(n-1)^2}{8R^2} + \frac{(n-1)(n-3)}{8}\left\{\frac{1}{r^2} - \frac{1}{\{R\sinh(r/R)\}^2}\right\}$$

In particular when $n = 3$ it is constant and so :

$$a_k(x,y) = (-2R^2)^{-k}\int_0^1\cdots\int_0^{r_{k-1}} dr_k \ldots dr_1 = \frac{1}{k!}(-2R^2)^{-k},$$

which is just the kth term in the power series expansion of $\exp\left(\frac{-1}{2R^2}\right)$,

which is what you would expect from the exact formula in Theorem (7.12) .

In general the scalar curvature S is given by , $-\frac{n(n-1)}{R^2}$.

So observe that in this special case of hyperbolic n-space we have :

$\frac{\Delta\theta_y(y)}{2\theta_y(y)} = \frac{S(y)}{12}$, as pointed out in (7.21) .

§8 Some Remarks about Elementary Formulae for Kernels of More General Operators

(8.0) In §7 we proved elementary formulae exhibiting small time asymptotic behaviour of kernels of elliptic operators $\mathbb{L}$ under a no-caustics assumption . This corresponds to elementary formulae exhibiting small μ asymptotic behaviour of kernels of elliptic operators of the form $\mu^2\mathbb{L}$. So the question arises , motivated in part by the work of **Mizrahi** [1] , **Davies and Truman** [1] and [2] , and **Fujiwara** [1] and [2] , whether we can derive elementary formulae exhibiting small μ asymptotic behaviour for our more general operators $\mathbb{K}^\mu$: this would include the small $\hbar$ asymptotics of Schrödinger Semigroups (even in a magnetic field) . Unfortunately this program has not been completed but I will give two simple examples that nevertheless indicate the problems that arise and make a number of conjectures .

(8.1) Gaussian Operators on $\mathbb{R}^d$

We take $\mathbb{K}^\mu$ on $\mathbb{R}^d$ of the form :

$$\frac{\mu^2}{2}\sum_{i,j=1}^{d} a_{ij}\frac{\partial^2}{\partial x^i\partial x^j} + \sum_{i=1}^{d}\Big(\sum_{j=1}^{d} b_{ij}x^j + c_i\Big)\frac{\partial}{\partial x^i}$$

where $a = (a_{ij})$ is a constant positive semidefinite matrix , $b = (b_{ij})$ is an arbitrary constant matrix and $c = (c_i)\in\mathbb{R}^d$.

(8.2) Hypoellipticity of Gausian operators on $\mathbb{R}^d$

We refer to chapter 15 by Chaleyat-Maurel and Elie in **Azencott et al** [1] for the following fact : K^μ is hypoelliptic if and only if the dxd^2 matrix $[a|ba|\ldots\ldots|b^{n-1}a]$ has rank d . We assume that our K^μ is hypoelliptic .

(8.3) Remark

Notice that this class of operators include the Ornstein Uhlenbeck Operator for which a=I , the identity matrix , b is the diagonal matrix $(-\lambda_1, \ldots, -\lambda_d)$ and c=0 .

(8.4) The Classical Mechanics of Gaussian Operators

(8.4.1) Firstly notice that the hypoellipticity condition of (8.2) is (H3) of (3.15) and so (3.16) and (3.21) imply that we have a correspondence between the associated Hamiltonian and Lagrangian Mechanics .

(8.4.2) The Hamiltonian $H:\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ governing the classical mechanics is :

$$H(p,q) = \frac{1}{2} \sum_{i,j=1}^{d} a_{i,j} p_i p_j + \sum_{i=1}^{d} \Big(\sum_{j=1}^{d} b_{i,j} q^j + c_i \Big) p_i .$$

Thus Hamilton's Equations are :

$$\frac{dq_i}{dt}(t) = - \sum_{j=1}^{d} b_{i,j} p_j(t) ,$$

$$\frac{dq^i}{dt}(t) = \sum_{j=1}^{d} a_{i,j} p^j(t) + \sum_{j=1}^{d} b_{i,j} q^j(t) + c_i ,$$

or equivalently :

$$\frac{dp}{dt}(t) = - b^T p(t) ,$$

$$\frac{dq}{dt}(t) = ap(t) + bq(t) + c .$$

So :

$$p(t) = \exp(-tb^T)p(0) , \text{ and}$$

$$q(t) = \exp(tb)q(o) + \int_0^t \exp((t-s)b) (a \exp(-sb^T) p(0) + c) ds$$

So we have a unique classical path from x to y in time t which is given by taking $p(0) = \exp(tb^T)K^{-1}(t)v(t,x,y)$, where :

$$K(t) = \int_0^t \exp((t-s)b) a \exp((t-s)b^T) ds , \text{ and}$$

$$v(t,x,y) = y - \exp(tb)x - \int_0^t \exp((t-s)b) c ds .$$

$K(t)$ is $K(t,h)(x)$ and $v(t,x,y)$ is $v_y(x)$ of (3.23) in this special situation : so $K(t)$ is indeed invertible by (3.16) . In fact from Chaleyat-Maurel and Elie in Chapter 15 of **Azencott et al** [1] we have :

(8.4.3) K^μ is hypoelliptic if and only if $K(t)$ is invertible .

(8.4.4) The action of this classical path is given by (3.23) as :

$$S(t,x,y) = \tfrac{1}{2}\, v(t,x,y)^T K^{-1}(t)\, v(t,x,y)$$

(8.5) Remark

Observe that for a invertible and $g = a^{-1}$ we have :

(8.5.1) If $b = 0$ and $c = 0$ then $v(t,x,y) = \exp_y^{-1}x$ with respect to the Riemannian structure g , $K(t) = ta$ and $K^{-1}(t) = g/t$, and generally

(8.5.2) $$|\det_g K(t)|^{-1} = |\det_g T_x\theta_t\Pi_t^{-1}|\exp\Big(-\int_0^t (\operatorname{div}_g Y)(\Pi\theta_s\Pi_t^{-1}x)\, ds\Big),$$

where Y is given by $Y_i(q) = \sum_{j=1}^{d} b_{i,j}q^j + c_i$, in standard coordinates .

Compare this with (4.10) .

(8.6) Elementary Formula for the Kernel of Gaussian Operators on $\mathbb{R}^d$

If g is an arbitrary Riemannian metric on $\mathbb{R}^d$ then the kernel with respect to the Riemannian measure is given by :

$$p^\mu(t,x,y) = \frac{1}{(\sqrt{2\pi\mu^2})^d}\,\frac{1}{\sqrt{|\det_g K(t)|}}\exp\Big(-\frac{v(t,x,y)^T K^{-1}(t)\, v(t,x,y)}{2\mu^2}\Big)$$

(8.7) Remarks

Observe that $v(t,x,y) \to x-y$ as $t \to 0$.

(8.8) A Conjecture

We make the following conjecture inspired by §6 and the above example :

In the situation of (3.23) let $K(x,y,t) = K(t,h)(x)$ and $S(t,x,y) = S_t(x)$. Choose a Riemannian metric g on M then the kernel with respect to the Riemannian Measure of K^{μ} , which is of the form $\mu^2 L + Y + W$, where L is expressed in Hörmander form as $\frac{1}{2}L_X^2 + X_o(X) + U$ is given by :

$$p^{\mu}(t,x,y)$$

$$= \sqrt{(2\pi\mu^2)^d}\, \varphi(t,x,y)\exp\left(-\frac{S(t,x,y)}{\mu^2} \right)E_x\left[\exp\left(\int_0^t \mu^2(\varphi_{u,t-u}^{-1} L \varphi_{u,t-u})(x^{t,\mu}(u))du\right)\right]$$

where :

$$\varphi(s,q,y) = \sqrt{|\det_g K(s,q,y)|^{-1}}\, \exp\left\{\int_0^t W(\gamma(u)) + \langle \rho(u), X_o(X)(\gamma(u))\rangle du\right\}$$

with $\rho(u)$ the solution of Hamilton's Equation and $\gamma(u)$ its projection onto M with the boundary conditions $\gamma(o) = q$ and $\gamma(s) = y$, and $x^{t,\mu}(u)$ is the solution of the following Stratonovich stochastic differential equation :

$$dx^{t,\mu}(u) = \mu X(x^{t,\mu}(u))dB(u) + \mu^2 X_o(X)(x^{t,\mu}(u)) + Y(x^{t,\mu}(u))$$

$$-A(dS_{u,t-u})(x^{t,\mu}(u)) + \mu^2 A(d\log\varphi_{u,t-u})(x^{t,\mu}(u))$$

$$dx^{t,\mu}(0) = x$$

See (8.14) for a discussion of the problems involved in proving this conjecture .

(8.9) 'Harmonic Oscillator' Operator on $\mathbb{R}^d$

We take K^μ on $\mathbb{R}^d$ of the form :

$$\frac{\mu^2}{2}\sum_{i,j=1}^{d} a_{i,j}\frac{\partial^2}{\partial x^i \partial x^j} - \frac{1}{\mu^2}\sum_{i=1}^{d}\Big(\frac{1}{2}\sum_{j=1}^{d} a_{i,j}x^i x^j + \sum_{j=1}^{d} a_{i,j}c^i x^j\Big)\frac{\partial}{\partial x^i}$$

where $a = (a_{i,j})$ is a constant positive definite matrix and $c = (c^i) \in \mathbb{R}^d$.

(8.10) Classical Mechanics of the 'Harmonic Oscillator' Operator

(8.10.1) The Hamiltonian $H: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ governing the classical mechanics is :

$$H(p,q) = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}p_i p_j - \sum_{i,j=1}^{d}\Big(\frac{1}{2}a_{i,j}q^i q^j + a_{i,j}c^i q^j\Big).$$

Thus Hamilton's Equations are :

$$\frac{dp_i}{dt}(t) = \sum_{j=1}^{d} a_{i,j}(q^j(t) + c^j),$$

$$\frac{dq^i}{dt}(t) = \sum_{j=1}^{d} a_{i,j}p^j(t),$$

or equivalently :

$$\frac{dp}{dt}(t) = a(q(t) + c),$$

$$\frac{dq}{dt}(t) = ap(t).$$

So :

$p(t) = \cosh(ta)p(0) + \sinh(ta)(q(0) + c)$, and

$q(t) = \sinh(ta)p(0) + \cosh(ta)(q(0) + c) - c$

Thus we have a unique classical path from x to y in time t which is given by taking $p(0) = \sinh(ta)^{-1}[(y + c) - \cosh(ta)(x + c)]$.

(8.10.2) If $g = a^{-1}$ then we have :

$$\emptyset(t,x,y) = |\det_g T_x\theta_t \pi_t^{-1}| = |\det_g \sinh(ta)|^{-1}$$

Compare with (4.10) .

(8.10.3) The Action of this classical path is given by :

$$S(t,x,y) = \tfrac{1}{2}(x-y)^T \tanh(ta)^{-1}(x-y) + 2(x + c)^T \sinh(\tfrac{1}{2}ta)(x + c)$$

(8.11) Elementary Formula for the Kernel of the 'Harmonic Oscillator' Operator

If g is the natural Riemannian metric given by a^{-1} then the kernel of K^μ with respect to the Riemannian measure is given by :

$$p^\mu(t,x,y) = \sqrt{(2\pi\mu^2)^{-d}}\sqrt{|\det_g \sinh(ta)|^{-1}} \exp\left(-\frac{S(t,x,y)}{\mu^2}\right) .$$

(8.12) Remark

Observe that $S(t,x,y) \sim \dfrac{d(x,y)^2}{2t}$ and $\emptyset(t,x,y) \sim t^{-d}$ as $t \to 0$,

where d is the Riemannian distance between x and y .

(8.13) Another Conjecture

We make the following conjecture motivated by the above example and §6 :

If L is elliptic then the kernel of K^μ , in its general form , with respect to the Riemannian measure given by the natural Riemannian

Elementary Formula because of the differing representations of $\varphi(t,x,y)$ and the 'Conditioned' process.

(8.14.2) It is not clear that the integrand inside the expectation is well defined for $\varphi(t-u,q,y)$ has a singularity as $u \to t$ so you have to show that the apparent singularities in the numerator and the denominator cancel each other out which is certainly the case if $\varphi(s,q,y)$ has its s and q variables seperable as occured in §7.

(8.14.3) We must prove an analagous theorem to (7.5) for this more general situation.

(8.14.4) Also we must show that $x^{t,y}$ is a bridge process that is a generalisation of (7.11).

(8.14.5) Given (8.14.2) to (8.14.4) we could attempt to prove the conjectures as in §7 and of course even try for higher order formulae in the same way.

(8.14.6) Also even in the case $M = \mathbb{R}^d$ with $L = \frac{1}{2}\Delta$, $Y = 0$, $W = 0$ there remains the question of the relationship between these conjectures and the results of **Mizrahi** [1] and **Davies and Truman** [1] and [2] where things are expressed in terms of Feynman Green's Functions.

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